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REFUELING AND EVAPORATIVE EMISSIONS OF VOLATILE ORGANIC COMPOUNDS FROM GASOLINE POWERED MOTOR VEHICLES

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by

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The United States Environmental Protection Agency has estimated that over 111 million people reside in areas that exceed the National Ambient Air Quality Standards for ozone. One major source of the chemical precursors (nitrogen dioxides and volatile organic compounds (VOCs)) for ozone are motor vehicles. The overall goal of this research is to improve the knowledge base related to VOC refueling and evaporative emissions from motor vehicles. Refueling, running loss, hot soak, and diurnal loss total and speciated VOC emissions were investigated.

A total of 12 uncontrolled refueling events were completed and involved the determination of volumetric flow rates of gasoline vapor during refueling, as well as total and speciated VOC concentrations. Total VOC emissions were compared with two commonly used algorithms. Speciated VOC vapor profiles were compared with two published gasoline vapor profiles and theoretical predictions based on knowledge of

liquid composition and environmental conditions. An evaluation of refueling emissions impacts on ozone formation potentials using MIR was completed and results were compared against speciated emissions and MOBILE-based total VOC emissions estimates coupled with a default speciation profile. Refueling VOC emissions and resultant ozone formation potential may be underestimated in existing emission inventories, particularly during the summer ozone season,

A model was developed to predict the speciation of VOCs associated with evaporative emissions from motor vehicles. Model-predicted speciation profiles were evaluated using SHED studies. Running loss, hot soak and diurnal emissions were included in each test. Total VOC emissions measured during each test were compared against MOBILE6 predicted emissions. An evaluation of evaporative emissions impacts on ozone formation potentials using MIR was completed, comparing measured and predicted emissions. The measured:predicted speciation results ranged between 0.93 and 1.11 and had an average value of 1.02. For the conditions tested, MOBILE6 underestimated evaporative emissions in 20 of 24 comparisons. MOBILE6-based ozone formation potentials may be underestimated.

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1. INTRODUCTION

1.1. The Problem

Negative impacts associated with poor air quality within the United States have been recognized for several decades. A major step to alleviate air pollution problems was taken in 1970 with the formation of the Environmental Protection Agency (EPA) and the passage of The Clean Air Act Amendments (CAAA) which, for the first time, established National Ambient Air Quality Standards (NAAQS) for several air pollutants. In addition, New Source Performance Standards (NSPS) were created to regulate emissions from various sources such as power plants and volatile organic liquid storage vessels. Over the past three decades, there have been two subsequent CAA amendments (1977 and 1990) involving the inclusion of several additional emissions sources (by 1992 over 70 different sources were regulated under NSPS) and increasingly more stringent emissions control levels in an attempt to reduce air pollution from these sources. Compounds for which NAAQS now exist include carbon monoxide, nitrogen dioxide, sulfur dioxide, ozone, particulate matter, and lead.

Although great strides have been made in improving air quality associated with air pollutants such as nitrogen dioxide, the EPA has estimated that over 111 million people continue to reside in 32 urban areas within the United States that exceed the NAAQS for ozone (United States Environmental Protection Agency Green Book, 2007). In 1997, the EPA promulgated a revised ozone standard based on an 8-hour average

concentration. Areas were classified as being in nonattainment with the new standard if the three year rolling average of the annual fourth highest 8-hour average ozone concentration exceeded 0.08 ppmv. In June of 2007, a new 8-hour ozone standard of 0.070 – 0.075 ppmv was proposed (United States Environmental Protection Agency Ozone Air Quality Standards, 2007)

As a basis for proposing the new 8-hour standard EPA cited information from studies which determined that there are several health impacts associated with high ozone concentrations. These range from reduced pulmonary function, throat irritation, chest pain to bronchoconstriction. In addition, these studies indicated that while not all people may be afflicted with these symptoms, there are "at-risk" groups including children, outdoor-workers, and individuals with pre-existing respiratory diseases, e.g., asthma. The intent of the new standard was to increase the level of protection for these at-risk populations against the potential health hazards associated with exposure to ozone.

Reduction of ozone concentrations to acceptable levels has proven to be extremely difficult. Part of the difficulty lies in the fact that ozone is not released directly into the atmosphere but is formed as a result of photochemical reactions involving sunlight and two major categories of chemical emissions, oxides of nitrogen (NO_x) and volatile organic compounds (VOCs).

Although a detailed descriptive analysis of the myriad of chemical reactions involved in ozone formation is beyond the scope of this dissertation, a simplified qualitative description of the basic chemical reactions is warranted in order to introduce the important role that VOCs have on ozone formation. Reactions 1-1 through 1-3

present the formation of ozone (O_3) resulting from the photolysis of NO_2 and subsequent potential cycling of NO, NO_2 and O_3.

$$NO_2 + h\nu \rightarrow NO + O \quad (1\text{-}1)$$

$$O + O_2 \rightarrow O_3 \quad (1\text{-}2)$$

$$O_3 + NO \rightarrow O_2 + NO_2 \quad (1\text{-}3)$$

VOCs participate in the enhanced formation of ozone through the interruption of the cycle established in Reactions 1-1 through 1-3. This is mediated via the generation of reactive peroxy radicals as denoted by $RO_2\cdot$, which ultimately result from reactions involving O and H_2O (Reactions 1-4, 1-5, and 1-6) and their ability to react with NO as presented in Reaction 1-7.

$$O + H_2O \rightarrow 2OH\cdot \quad (1\text{-}4)$$

$$OH\cdot + R\ (VOC) \rightarrow R\cdot + H_2O \quad (1\text{-}5)$$

$$R\cdot + O_2 \rightarrow RO_2\cdot \quad (1\text{-}6)$$

$$RO_2\cdot + NO \rightarrow RO\cdot + NO_2 \quad (1\text{-}7)$$

The generation of radicals from VOCs allow for NO $\rightarrow NO_2$ (Reaction 1-7) and the subsequent maintenance of a "driving force" for Reactions 1-1 and 1-2 without passing through Reaction 1-3. This alternative path for NO $\rightarrow NO_2$ bypasses the destruction of O_3 which results from Reaction 1-3, thereby elevating levels of O_3. However, not all VOCs participate equally in this chemical reaction process. It is this difference in VOC reactivity that necessitates an understanding of total VOC composition in order to be able to predict/control ozone formation.

One major source of both NO_x and VOC emissions are motor vehicles. Emissions data released by the USEPA indicate that on road gasoline-powered vehicles are responsible for approximately 19 and 23% of the total anthropogenic NO_x and VOC emissions, respectively (United States Environmental Protection Agency, 2003a). While motor vehicle NO_x emissions are products of combustion, VOC emissions result from both incomplete fuel combustion (exhaust) and evaporative losses of fuel.

Fuel consumption data indicate that Americans use, on average, approximately 1.9 gallons/licensed driver/day (National Petroleum News, 1995). Daily average throughput of gasoline at an average U.S. service station has been estimated to be approximately 2,000 gallons (Shedd, S. A., 1992). On a vehicle basis, EPA has estimated that there are approximately 180 million gasoline-powered vehicles operating in the national fleet resulting, in an average total annual travel distance of over two trillion miles (United States Environmental Protection Agency, 1999a). Given the magnitude of

fuel consumption, number of vehicles, and annual miles traveled, it is obvious why motor vehicles are a significant contributor to air pollution.

The relative significance of evaporative emissions of VOCs has increased since 1970. This is primarily the result of increasingly stringent limits placed on VOC emissions. For example, in 1970 when VOC exhaust emissions were first regulated with the introduction of a 0.41 gram VOC/ mile (g/mi) limit for new vehicles, uncontrolled VOC exhaust emissions were estimated to be approximately 13 g/mi (United States Environmental Protection Agency, 1994a). In 1994, certification exhaust VOC emissions for new vehicles was 0.25 g/mi. The relative significance of exhaust and evaporative VOC emissions was assessed as part of the 1998 NARSTO Mobile Sources Critical Review (Sawyer *et al*., 1998). Exhaust:evaporative emission ratios were reported to be temperature dependant and ranged from 2.4:1 at 75 °F to 0.7:1 at 105 °F. Therefore, for states such as Texas that have high average summer temperatures, the relative importance of evaporative emissions make this source a potentially significant contributor to degradation of air quality in urban areas.

1.2. Research Objectives

The overall objective of this dissertation is to improve the knowledge base related to VOC evaporative emissions from motor vehicles. Total and/or speciated VOC emissions generated from the following four motor vehicle evaporative sources were investigated:

- Refueling

- Running losses
- Hot soak
- Diurnal.

Improved estimates of VOC emissions from these sources will be of use in the assessment of current information used in relation to motor vehicle evaporative emissions and refinement/development of both total and speciated VOC emission inventories that are required for (1) air quality modeling, e.g., tropospheric ozone, and (2) comparing measured urban air toxic concentrations with source-specific speciated emissions to determine which sources are significant contributors of air toxics.

Specific objectives of this research included:

1. Measure "in-use" uncontrolled vehicle refueling emissions (both total and speciated VOCs).
2. Use Objective 1 results to assess the accuracy of several commonly-used total VOC refueling emissions algorithms.
3. Develop an emissions speciation model for diurnal, hot soak and running loss evaporative emissions.
4. Evaluate the emissions speciation model using Sealed Housing for Evaporative Determination (SHED) experimental data.
5. Assess the significance of speciated refueling and evaporative emissions on potential ozone formation.

1.3. Scope of Research

This dissertation involved two major components (analysis of refueling and evaporative emissions), each of which represent an original contribution to the field. Each component and associated tasks are summarized in Table 1-1.

Table 1-1. Major Components and Associated Tasks.

Field Measurement of uncontrolled refueling emissions
Design and construction of novel sampling device.
Completion of 12 sampling events.
Measurement of vapor flow rates.
Determination of liquid gasoline speciation profiles.
Speciation of pre-fill and refueling vapors.
Comparison of measured and predicted emissions.
Comparison of measured and predicted ozone formation potential.
SHED Tests to assess evaporative emissions
Design of experimental plan for SHED experiments.
8 SHED experiments (completed by external lab),
Comparison of measured and predicted emissions.
Development of VOC speciation model for evaporative emissions.
Comparison of measured and predicted speciations.
Comparison of measured and predicted ozone formation potential.

1.4. Organization of Dissertation

This dissertation is organized as follows: Background information on motor vehicle VOC emissions is presented in Chapter 2. Previously completed research related to motor vehicle evaporative emissions, including refueling, running losses, hot soak and diurnal emissions are discussed in Chapter 3 as well as algorithms currently used to estimate emissions associated with the various categories of evaporative emissions. Experimental methodologies developed and used during the completion of this work are presented in Chapter 4. Experimental results are presented in Chapter 5. Data presented in Chapter 5 are then used in Chapter 6 to demonstrate the potential impacts that the experimental results/findings may have on ozone formation. Conclusions and recommendations associated with this research are summarized in Chapter 7.

2. BACKGROUND

The USEPA has estimated that light duty gasoline vehicles are responsible for approximately 23 percent of total anthropogenic VOC emissions (United States Environmental Protection Agency, 2003a). There are two primary classifications of motor vehicle VOC emissions: exhaust and evaporative. Because of the relative significance of motor vehicles in terms of total VOC emissions, it is imperative that both the absolute and relative contributions of these source categories be understood.

Several studies have been completed which involved investigation of total VOC evaporative emissions (American Petroleum Institute, 1991; American Petroleum Institute, 1992; American Petroleum Institute, 1994; Brooks *et al*., 1995; Coordinating Research Council, 1997; Coordinating Research Council, 1998a; Coordination Research Council, 1998b). However, while these studies have significantly increased the knowledge-base related to total VOC evaporative emissions and factors that impact the quantity of emissions generated, e.g., fuel volatility and environmental conditions, there has been limited research performed in which the composition of evaporative emissions were investigated.

Information pertaining to speciation of evaporative emissions is important for at least two reasons. First, with the exception of a few compounds, e.g., methane, most VOCs are considered to be reactive and will participate in the formation of ozone through reaction pathways described previously. However, the relative reactivities of individual compounds are known to vary considerably. For example, using the ozone formation potential metric, Maximum Incremental Reactivity (MIR), developed by Carter (1998),

butene has the potential to generate more than seven times the amount of ozone than an equivalent mass of butane. Secondly, gasoline contains several compounds currently classified as hazardous air pollutants (HAPs, also commonly referred to as air toxics), some of which have been identified as known human carcinogens, e.g, benzene. Examples of other HAPs routinely detected in gasoline include ethylbenzene, isooctane, methyl-tert butyl ether, toluene, and xylenes. Several of these HAPs are present in gasoline at concentrations ranging from 1 to 10% by mass. In July of 1999, the USEPA (United States Environmental Protection Agency, 1999b) finalized the Integrated Urban Air Toxics Strategy, a plan designed to reduce emissions of 33 air toxics in urbanized areas. The EPA has estimated that motor vehicle emissions account for as much as half of all cancers attributed to outdoor sources of toxics. (United States Environmental Protection Agency, 1995a).

One method currently used for assessing the real world contribution and composition of motor vehicle emissions is through chemical mass balance (CMB) receptor modeling (Mugica *et al*., 1998; McLaren *et al*., 1996a). For a complete description of CMB modeling, it is recommended that the reader review Watson *et al*., (2001), as this reference provides an excellent overview of CMB modeling procedures, assumption and limitations.

Briefly, the CMB method involves a statistically-based comparative analysis of collected whole air sample composite speciations and source-specific speciation profiles. Typical sources included in CMB modeling include gasoline-powered motor vehicle exhaust and evaporative emissions, motor vehicle diesel exhaust emissions, industrial

emissions, refinery emissions and other source types considered significant for the area of concern, Source-specific profiles are combined in a manner to generate a total speciation profile similar to that measured. The actual combination of individual source profiles is done statistically using a least-squares resolution method. Once completed, the relative contribution of individual source profiles is obtained. In addition to providing valuable information related to relative contributions of individual emissions sources, CMB modeling can also be used to evaluate the relative contributions of emissions sources contained within emission inventories. For example, Fujita *et al*., (1995a) completed CMB work for the San Francisco Bay area and determined that motor vehicles averaged approximately 77.5% of the VOC emissions, with an exhaust:evaporative emissions ratio of 2.1:1. McLaren *et al*., (1996b) completed CMB work in the Cassiar tunnel, Vancouver, BC and determined that 63% of the exhaust emissions were associated with unburned gasoline, which has a significantly different profile than exhaust emissions.

However, it is important to note that other studies utilizing dynamometers and sealed housing for evaporative determination (SHED) testing have had different findings in terms of the relative significance of exhaust and evaporative emissions. For example, Pierson *et al*., (1997) reported that evaporative emissions exceeded exhaust emissions. Black *et al*., (1998) tested seven gasoline-powered motor vehicles and found that evaporative emissions made up 34 to 84% of total VOC emissions and were, on average, 25% higher than exhaust emissions.

Due to the difference in individual VOC reactivities and the associated impacts on ozone formation potential, an improved understanding of the quantities and composition

of evaporative emissions was the focus of this dissertation. The purpose of the research described herein is to advance the knowledge-base associated with both total and speciated gasoline-powered motor vehicle evaporative emissions.

2.1. Motor Vehicle Evaporative Emissions

There are generally considered to be five different sources or categories of evaporative emissions:

- Refueling
- Running losses;
- Hot soak;
- Diurnal; and
- Resting losses.

A summary of each of these sources is provided below.

2.1.1. Refueling Emissions

Refueling losses occur as a result of displacement of gasoline vapors from the gas tank as it is filled with fuel. The fate of the displaced vapors is dependent upon the vehicle being refueled and/or the area in which the refueling is occurring. Beginning in 1998 and utilizing a 40, 80, and 100% annual phase-in schedule, culminating in the model year 2000, all gasoline-powered passenger vehicles (defined as vehicles with gross vehicle weight < 6,000 lbs) are required to capture refueling emissions using an on-board refueling vapor recovery (ORVR) system. Refueling emissions for gasoline-powered

light duty trucks (defined as trucks with gross vehicle weights < 6000 lbs) are also covered under the ORVR regulation. Introduction of ORVR equipment on new light duty trucks was scheduled to commence in the model year 2001 and follow the same three year 40, 80, 100% annual phase-in schedule as that required for light duty vehicles. Due to the time required to achieve complete vehicle fleet turnover, full benefits associated with implementation of ORVR, i.e., control of all passenger vehicle refueling emissions, will not be obtained for approximately 25 years or 2023 (United States Environmental Protection Agency, 1994b). In terms of refueling emissions capture efficiency, ORVR has a default value of 98% efficiency as used in the MOBILE models. (United States Environmental Protection Agency, 2003b) .

Prior to 1998, vehicles were not designed to capture refueling emissions. Therefore, control of refueling emissions prior to ORVR, if required, was accomplished solely through "capture at the pump nozzle" technology. This technology, known as Stage II control, consists of passive or active control systems.

Passive Stage II control involves the passive collection and storage of displaced gasoline vapors within the service station gasoline tank. Vapors are collected in a large hose that encompasses the smaller liquid gas line as they are expelled from the fill-pipe. Because the collection of vapors is a passive process, dispensing of gasoline is not enabled until a tight seal is made between the vehicle fill-pipe area and the gasoline pump nozzle "boot".

Active Stage II control also utilizes the underground storage tank for vapor storage but uses a pump to vacuum-assist the capture of displaced vapors. As gasoline is

dispensed, a vacuum pump is activated which captures and "pulls" the displaced gas tank vapors through a vapor line surrounding the liquid gasoline supply line. The vapors are then pumped into a gasoline storage tank, most commonly located underground. To ensure that all displaced vapors are captured, the quantity of vapor pulled by the vacuum pump is in excess of the volume of displaced gas tank vapors. Due to the expense of these systems, Stage II control has generally only been implemented in areas designated as ozone nonattainment. For all other areas, and prior to 1998, all vehicle refueling was uncontrolled and the displaced vapors were simply emitted into the ambient atmosphere. Stage II efficiencies from operating gasoline refueling stations have been reported to range from 81 to 93% (MacIntosh *et al*., 1994). A similar study was done in Mexico City in which ten service stations were evaluated, resulting in measured Stage II efficiencies ranging from 82 to 99% with an average refueling emissions capture efficiency of 90%. (Cruz-Nunez *et al*., 2003).

2.1.2. Running Loss, Hot Soak, Diurnal and Resting Loss Emissions

Running loss evaporative emissions are generated during vehicle operation. As the vehicle is running, any fuel vapors that are not captured by the emissions control system are released. Vapors are generated as a result of the heating of fuel which may be caused by both environmental conditions and/or recirculation of the fuel through the fuel system, i.e., fuel injection systems only. In addition, it is also possible that running loss emissions occur as a result of fuel system leaks in either gasoline vapor or fuel lines, e.g.,

cracked hoses or loose hose fittings. During operation and under normal operating pressures, vapor or liquid gasoline may leak from the vehicle.

Hot soak emissions are defined as those emissions occurring in the first one-hour period after vehicle operation. As the vehicle cools down after operation gasoline vapors may be generated and released. These emissions are believed to occur mainly from fuel delivery sources such as carburetors or fuel injection systems which at the time of engine shut-off will have fuel present which can then evaporate over time due to high temperature.

Diurnal emissions are classified as emissions generated from parked vehicles, i.e., non-operating, during the diurnal ambient temperature cycle. As the ambient temperature increases, heat transfer to the fuel tank results in additional vapor formation. Diurnal emissions may occur as a result of a failure in the ability of the system to withstand gas tank pressurization, e.g., leaking gas cap, or reduced adsorptive capacity of the evaporative emissions control canister, both of which will result in the release of gasoline vapors.

Resting loss emissions are defined essentially as all other evaporative emissions not captured by running loss, diurnal or hot soak definitions and include losses from thermally-stable, i.e., no temperature gradient driving force for fuel vaporization, non-operated vehicles.

The EPA-approved method for quantifying emissions for each of the four categories listed above revolves around the use of a Sealed Housing Enclosure for Evaporative Determination (SHED) test system. While the exact protocols for each

evaporative emission test differ, the underlying principle of capturing all emissions within the enclosure is central to all tests.

For a detailed overview of SHED testing requirements, the reader is referred to the Code of Federal Regulations Title 40 Section 86 Control of Air Pollution From New and In-Use Motor Vehicles and New And In-Use Motor Vehicle Engines: Certification and Test Procedures (Code of Federal Regulations, 1993). Briefly, the test vehicle is contained within an enclosed environment during the testing period. Test enclosure VOC concentrations are measured prior to and at test-end in order to determine the increase in VOC concentration occurring over the test period. Emission rates are calculated as the product of the change in VOC concentrations and the volume of the test chamber. Major differences between the individual test procedures are:

- Running loss emissions are measured during operation of the test vehicle on a dynamometer within the SHED. The federal test sequence involves the completion of three individual Urban Dynamometer Driving Schedule cycles. These cycles have been developed to encompass typical driving patterns encountered in most urbanized areas.
- Hot soak emissions are quantified during the one-hour time period immediately after time of key-off. During this time the ambient temperature within the SHED is set to 95 °F.
- The diurnal emissions standard is based upon a test that involves three successive 24-hour diurnal cycles. The diurnal minimum and maximum temperatures are 72 and 96°F, respectively.

- Resting loss emissions are quantified during the last 6 hours of the diurnal test in which the vehicle and ambient temperatures have stabilized. As a result, diurnal and resting loss emissions are often lumped together and reported simply as diurnal losses.

A description of the evaporative emissions testing included as part of this research is included in Chapter 4. A summary of previous research related to refueling and evaporative (running loss, hot soak, and diurnal loss) emissions is presented in the next chapter.

3. PREVIOUS RESEARCH

This chapter is intended to provide a summary of past research related to refueling and evaporative emissions. Model algorithms are presented, along with a discussion of the limitations of previous research.

3.1. Refueling Emissions

Several earlier studies on total VOC emissions during uncontrolled refueling have been completed and are described below in chronological order. In some studies, sufficient data were obtained to facilitate development of a refueling emissions algorithm while for other studies only observations or trends were reported.

Smith (1972) reported the results of refueling tests performed using a mini-SHED, which is a structure designed to enclose a fuel-tank instead of the entire vehicle. During these experiments, fuel tanks with different configurations were refueled with gasolines of varying Reid vapor pressures (RVPs) during different temperature conditions. The refueling algorithm stemming from Smith's experiments is presented as Equation 3-1.

$$E = \exp(-0.02645 + 0.01155T_{DF} - 0.01226T_V + 0.002246T_V \times RVP) \quad (3\text{-}1)$$

Where:

E = refueling total VOC emissions (g / gallon of dispensed fuel)

T_{DF} = average dispensed fuel temperature (°F)

T_V = average tank vapor temperature (°F)

RVP = dispensed fuel RVP (psi)

Additionally, top-filled and bottom-filled experiments were completed. The results indicated that the maximum difference between refueling emissions associated with top- and bottom-filled were no more than 10 percent. These findings led the authors to determine that emissions associated with entrained fuel droplets being emitted during refueling were not significant, as these types of emissions would not be present during bottom-filled refueling.

Hochhauser and Campion (1976) also completed fuel tank refueling experiments similar to Smith (1972). One difference, however, is that all displaced vapors were captured in a Tedlar bag thus allowing for the quantification of mass of VOCs emitted and the volume of vapor displaced. By quantifying the volume of vapors emitted, impacts of temperature differences between the dispensed fuel and the tank could be examined to understand the phenomenon of vapor growth or shrinkage. By completing refueling experiments under conditions in which fuel RVP, dispensed fuel and tank temperatures were varied Hochhauser and Campion (1976) developed the following algorithm to predict refueling emissions:

$$E = \exp(-1.23 + 0.0185T_D + 0.00170T_T + 0.118RVP) \quad (3\text{-}2)$$

Where:

E = refueling total VOC emissions (g / gallon of dispensed fuel)

T_D = average dispensed fuel temperature (ºF)

T_T = average tank temperature (ºF)

RVP = dispensed fuel RVP (psi)

The following relationship between the volume of vapor emitted and volume of gasoline dispensed was also developed:

$$V/L = 1.0 + \Delta T\ (0.0102 - 0.000206T_T - 0.000888RVP) \quad (3\text{-}3)$$

Where:

V/L = volume of vapor emitted per volume of gasoline dispensed (gal vapor / gal liquid)

$\Delta T = T_T - T_D$ (ºF)

T_T, T_D and RVP as previously defined

Impacts of fuel delivery rates and the amount of fuel in the tank prior to refueling were also investigated by Hochhauser and Campion (1976) setting up a 2 x 2 factorial experiment involving flowrates of 5 and 10 gpm and initial tank fuel volumes of 5 and 10 gallons was employed. Results of these experiments indicated that the emission rates were not impacted by either the fuel flowrate or the initial tank volume.

Rothman and Johnson (1985) developed an uncontrolled refueling algorithm that currently serves as the uncontrolled refueling emissions factor in AP-42 (United States Environmental Protection Agency, 1995b). As such it has been incorporated into the family of motor vehicle emissions estimation models referred to MOBILE and approved for use in estimating motor vehicle emissions inventories by the USEPA. The algorithm was based on SHED studies involving 8 vehicles, 4 fuels of varying volatilities and varying dispensed fuel and tank temperatures. The algorithm developed was:

$$E = -5.909 - 0.0949\Delta T + 0.0884T_D + 0.485(RVP) \quad (3\text{-}4)$$

Where all parameters are as previously defined.

While Equation 3-4 is also based on the same parameters as other refueling algorithms, it is worthwhile noting that the emissions are described as being a linear function of ΔT, T_D and RVP, while all other algorithms contain an exponential relationship.

The MOBILE refueling algorithm, while taking on the same form as the AP-42 algorithm (Equation 3-4), requires ambient data instead of specific dispensed temperature and tank vapor temperature. The current version of MOBILE in use, MOBILE6, uses the same refueling algorithm as that previously described for the earlier version MOBILE5a and is:

$$E = -5.909 - 0.949*TDFDIF + 0.0884*DFTEMP + 0.485*RVP \quad (3\text{-}5)$$

Where:

TDFDIF = 0.418 * DFTEMP – 16.6

DFTEMP = AMBT

TDFDIF = difference between tank temperature and dispensed fuel temperature, (°F);

DFTEMP = dispensed fuel temperature (°F)

AMBT = ambient temperature (°F).

MOBILE6 has the following additional parameter constraints:

IF DFTEMP < 20, then DFTEMP = 20,

IF DFTEMP > 95, then DFTEMP = 95,

IF TDFDIF > 20, then TDFDIF = 20, and

IF DISPL < 1.8, then DISPL = 1.8

These changes in temperature data requirements facilitate the development of emissions estimates through the use of ambient temperature data which are easily obtainable. However, MOBILE6 does put upper limits on emissions as a result of these constraints, most notably the upper temperature of 95 °F for ambient and DFTEMP temperatures. In Texas ambient temperatures are often higher than this temperature during summertime conditions.

Braddock *et al*. (1986) performed SHED refueling tests on three different vehicles and measured total and speciated compound emissions. Although a refueling algorithm was not presented, several major findings associated with this research were provided. These included:

- Refueling emissions were not sensitive to liquid delivery rate. When emissions were normalized as mass VOC emitted per gallon dispensed, measured emissions ranged from 4.27 g / gal to 4.61 g / gal for delivery rates ranging from 2.0 to 8.0 gpm.
- Refueling emissions were not sensitive to fuel tank capacity or vehicle refueling system geometry or configuration. Three different vehicles (1976 Ford Mustang, 1976 Dodge Ram Pickup and 1985 Chevrolet Caprice) when refueled during three tests using the same fuel delivery rate and RVP gasoline (8.0 gpm,11.4 psi) and identical fuel dispensed and fuel tank temperatures (59 ºF and 73 ºF, respectively) had average refueling emissions that ranged from 4.51 to 4.54 g / gal.
- Refueling emissions were primarily due to vapors resident in the fuel tank prior to refueling. This was based on experiments in which either gasoline or water was

delivered to a tank containing 2 gallons of gasoline. Emissions associated with the water-dispensed tests were only 13 percent less than for the gasoline-dispensed test, (3.95 g / gal vs. 4.54 g / gal).

- Dispensed fuel and fuel tank temperatures impacted refueling emissions. When the dispensed fuel temperature was lower than fuel tank temperature, vapor shrinkage was reported. Conversely, when the dispensed fuel temperature was higher than the fuel tank temperature, vapor growth occurred.
- The authors did discuss the concept of fuel aging and its potential impacts on refueling emissions, and stated that this would be studied further in a follow-up research study (discussed later in this section).

It is important to note that although the authors describe the impacts of dispensed fuel and fuel tank temperatures using the terms vapor "shrinkage" and "growth", the actual volume of vapors emitted during vehicle refueling was not measured. Instead, it appears that the term vapor growth or shrinkage is simply related to the relative increase or decrease in mass emissions to a standard condition (dispensed fuel temperature of 59 ºF and fuel tank temperature of 85 ºF).

Furey and Nagel (1986) completed two refueling experiments that differed from all other studies discussed above in that they performed tests that involved the use of different tank and dispensed fuels. Their findings indicated that the refueling vapor speciation was impacted by type of fuel dispensed, and not simply related to displaced fuel tank vapors. Although only two tests were completed, it was suggested that based on

fuel compositions, the refueling vapor composition appeared to consist of 35 percent fuel tank vapor and 65 percent dispensed fuel-related vapors.

In the follow-up study to Braddock *et al.*(1986), Braddock (1987) completed a total of 27 SHED refueling experiments involving one vehicle, three fuels with varying volatilities (RVPs ranging from 10 to 13.3 psi) and different tank (40 to 108ºF) and fuel delivery temperatures (50 to 88 ºF). The following algorithm was developed based on experimental data:

$$E = 1.225 - 0.0476\,\Delta T - 0.0592\,T_D + 0.153RVP \qquad (3\text{-}6)$$

Where all parameters are as previously defined.

Braddock (1987) presented some speciation data facilitate the understanding of how different refueling conditions may impact the speciation profile. It was reported that the speciation profiles were actually independent of temperature or fuel type. Refueling vapors were primarily comprised of alkanes (80%), olefins (15%) and aromatics (5%).

Cingle and McClement (1988) developed an empirical algorithm for estimating VOC emissions during uncontrolled vehicle refueling. Their study consisted of 445 individual refueling experiments, 22 different vehicles, three different fuels (RVPs of 8.8, 10.3 and 11.6 psi), three different fuel delivery temperatures (70, 80 and 88 °F), and three different fuel and tank temperature differences (ΔT of +10, 0, and -10 °F). The resulting algorithm developed is shown here as Equation 3-7:

$$E = \exp(-1.2798 - 0.0049\Delta T + 0.0203T_D + 0.1315RVP) \qquad (3\text{-}7)$$

Where all parameters are as previously defined. Equation 3-7 was used as the basis for determining baseline emissions for the On-Board Refueling Vapor Recovery (ORVR)

Standard Final Regulatory Impact Analysis (USEPA, 1994b). As such, it has been used during the evaluation of on-board carbon canister designs and subsequent residual emissions associated with ORVR. Should this equation underestimate refueling emissions, it is possible that the required sizing of ORVR systems could also be underestimated, resulting in higher residual emissions occurring as a result of emissions breakthrough.

3.1.1. Limitations of Previous Refueling Emissions Research

Although several studies have been completed to quantify refueling emissions and have led to development of refueling emissions algorithms, none of these studies have developed algorithms for conditions that have dispensed fuel that is different than the tank fuel. This difference in fuel composition may impact refueling emissions as "fresh" fuel that is dispensed into "aged" fuel within the tank will differ in individual compound concentrations, and thus drive liquid-to-vapor mass transfer as the dispensed fuel is introduced in the fuel tank.

In order to better understand this potential impact, this dissertation research involves the speciation of resident tank vapors immediately prior to refueling, the speciation of displaced vapors during refueling, and the quantification of displaced vapors. To accomplish this, unique sampling equipment was designed and used to capture displaced tank vapors during uncontrolled refueling. Dispensed fuel liquid composition has also been characterized during each refueling experiment to facilitate an

understanding of the impacts of dispensed fuel composition on refueling vapor composition. Details related to experimental methods are presented in Section 4.1.

3.2. Evaporative Emissions

For several years it has been understood that motor vehicle evaporative emissions may be a significant contributor in terms of total VOC emissions. As early as 1967, studies were completed to determine impacts of fuel RVP and temperature conditions on carburetor losses (Wade, 1967). Several studies have been undertaken to quantify evaporative emissions from in-use vehicles using controlled SHED tests (Haskew *et al*., 1990; Brooks *et al*., 1995, Coordinating Research Council, 1997; Coordinating Research Council, 1998a; Coordination Research Council, 1998b). Many of these studies have been used to develop algorithms used in MOBILE6 for predicting running loss, hot soak and diurnal total VOC emissions (USEPA, 1999a; USEPA, 1999c; USEPA, 1999d; USEPA, 2001). Algorithms contained in MOBILE6 have been developed to predict emissions as a function of several parameters such as vehicle age, fuel delivery system, i.e., fuel injected vs. carburetors, fuel RVP and temperature. As an example, diurnal emissions are predicted using the following equation:

$$E = A + B*RVP + C*(MEANVP * DELVP) + D*(MEANVP*DELVP)^2/ 1000 \quad (3\text{-}8)$$

Where

E = diurnal emissions (g VOC/day-vehicle)

A, B, C and D are vehicle age, fuel system-specific and evaporative system pressure test result-specific coefficients

RVP = Reid vapor pressure of gasoline (psi)

MEANVP = mean gasoline vapor pressure (kPa)

DELVP = hourly high temperature gasoline vapor pressure – hourly low temperature gasoline vapor pressure (kPa)

For a detailed review of this and other algorithms developed for hot soak and running loss emissions, the reader is referred to the references previously cited (USEPA, 1999a; USEPA, 1999c; USEPA, 1999d; USEPA, 2001).

In recognition that there are also motor vehicles that have evaporative emissions associated with liquid gasoline leaks, MOBILE6 also has algorithms for predicting both the frequency of vehicles that are liquid leakers, termed Gross Liquid Leakers, and the quantity of total VOC emissions released from these vehicles. Information on how this category of evaporative emissions is quantified can be found in USEPA (1999e).

Concerns over motor vehicle evaporative emissions have not been limited to the United States. For example, in Australia, Duffy *et al*. (1999) completed experiments to determine hot soak and heat build (referred to as diurnal losses in the United States) emissions associated with different vehicle ages, fuel types and temperatures. They found that evaporative emissions from older vehicles, as defined as pre-1985 were 2-3 times higher than newer vehicles (post-1985).

Van der Westhuisen *et al*. (2004) investigated evaporative emissions from motor vehicles in South Africa using similar testing procedures as those utilized in the United

States, e.g., Sealed Housing for Evaporative Determination or SHED. Temperatures tested were as high as 40 °C (104 °F), comparable to temperatures encountered in Texas during the summer season. Results indicated that the South African vehicle fleet, which at the time of the report were not required to control evaporative emissions, had emissions ranging from 10 to 50 times higher than those for similarly-aged vehicles regulated elsewhere.

3.2.1. Speciated Evaporative Emissions

Concerns related to emissions of toxic compounds from gasoline, e.g., benzene, have motivated several studies to understand the impacts that different fuel volatilities and environmental conditions may have on the evaporative emissions of these compounds (Seizinger *et al*., 1986; Sigsby *et al*., 1987; Stump *et al*., 1990; Burns *et al*., 1992; Reuter *et al*., 1992; Stump *et al*., 1992; Gabele and Knapp, 1993; Koehl *et al*., 1993; Reuter *et al*., 1994; Stump *et al*., 1994). While these studies have led to compound-specific results, e.g., temperature or liquid gasoline compound concentration impacts on emissions, there is a paucity of studies that contain sufficient data to facilitate the development and confirmation of a predictive model for estimating vapor speciation as a function of liquid composition, temperature and fuel volatility.

3.2.2. Limitations of Previous Evaporative Emissions Research

Significant research has been done to understand how total VOC evaporative emissions, i.e., running loss, hot soak, and diurnal, are impacted by vehicle, environmental and fuel conditions. The USEPA has developed the MOBILE6 model to

facilitate the development of motor vehicle emissions inventories. These inventories, when coupled to speciation profiles, can then be used in photochemical ozone formation modeling to predict impacts of VOC emissions on local airshed ozone concentrations.

One problem associated with this methodology is the routine reliance on default gasoline vapor speciation profiles as area-specific profiles are not available. To facilitate an improvement in the current practice of developing speciated emission inventories, one component of this dissertation was to develop a speciation model (TEVAP) that, given fuel RVP, temperature conditions and liquid gasoline speciation, can predict vapor speciation profiles. The speciation model predictions were compared to measured evaporative speciated emissions obtained under varying test conditions in this study. The model is described in Appendix B. A comparison of predicted and measured speciation results is presented in Section 5.2.4

4. EXPERIMENTAL METHODOLOGIES

Two different groups of experiments were performed during the completion of this research. The first was designed to quantify VOC emissions that occur during the refueling of vehicles. The second group was designed to quantify non-exhaust emissions that occurred as a result of vehicle operation/rest. The type of emissions associated with the second group of experiments has collectively been called evaporative emissions. The methods/procedures used during the completion of these experiments are described below.

4.1. Uncontrolled Refueling Emissions

4.1.1 Overview

Total VOC and speciated compound emissions were measured during uncontrolled vehicle refueling. Twelve vehicle refueling events were performed during which emissions were determined by the product of vapor flow rate and VOC concentration. Vehicles filled and service station locations are listed in Table 4.1. All experiments were completed in Austin, which does not have mandated Stage II recovery. Vehicles selected for use in these experiments did not have on-board vapor recovery devices.

Uncontrolled refueling emissions were measured by routing displaced tank vapors through a vapor sampling and flow rate measurement apparatus. Vapor samples were

collected in glass sampling bulbs and analyzed for concentrations of both speciated and total VOCs. Vapor flow rates were obtained by the collection of displaced vapors in a plastic bag. The volume of vapor collected and the amount of gasoline dispensed during the period of vapor collection were used to determine vapor flow rate, expressed as volume of vapor displaced/ volume of gasoline dispensed.

Table 4.1. Vehicle Refueling Experiments.

Experiment	Vehicle	Service Station
1	1987 Toyota Corolla	Chevron
2	1991 Chevrolet Blazer	Chevron
3	1993 Oldsmobile Achieva	Chevron
4	1991 Chevrolet Blazer	Chevron
5	1993 Oldsmobile Achieva	Chevron
6	1991 Chevrolet Blazer	Chevron
7	1991 Chevrolet Blazer	UT
8	1991 Chevrolet Blazer	UT
9	1991 Chevrolet Blazer	UT
10	1991 Chevrolet Blazer	UT
11	1991 Chevrolet Blazer	UT
12	1991 Chevrolet Blazer	UT

Chevron = Chevron service station located on Burnet Road in Austin, Texas.
UT = University of Texas at Austin, J. J. Pickle Research Campus Refueling Facility.

Various parameters were measured during each refueling experiment. These included dispensed liquid gasoline temperature, displaced vapor temperature, and gasoline pump rate. In addition, dispensed gasoline samples were collected in order to characterize Reid vapor pressure (RVP) and chemical composition. Measured total VOC emission rates were compared to two commonly used emission algorithms for gasoline refueling.

4.1.2. Specific Refueling Emissions Methods

Sample Collection: Liquid

During each refueling experiment a dispensed gasoline sample was collected to allow for the characterization of RVP and chemical composition. Sample collection, preservation, and analysis protocols are described below.

Sample Collection

Liquid samples were collected by dispensing gasoline into 500 mL glass vials. Each vial was filled with approximately 400 mL of gasoline and then sealed using an O-ring fitted screw-cap with Teflon backing to maintain air-tightness. Samples were stored on ice during transport to The University of Texas at Austin (UT). Upon return to UT, samples were refrigerated until Reid Vapor Pressure (RVP) analyses were completed.

Density Analysis

Density measurements were made using the following protocol

1. An empty 2 mL vial was labeled, capped and weighed.
2. One (1) mL of gasoline at room temp (approximately 75 °F) was injected into the weighed vial and the vial was capped.
3. The vial was reweighed. The difference in weight was divided by 1 mL to determine the density.

Reid Vapor Pressure Analysis

Reid vapor pressure (RVP) measurements were performed on all samples. Values of RVP were determined using the American Society for Testing and Materials (ASTM) test method procedure Standard Test Method for Vapor Pressure of Petroleum Products (Reid Method) D-323. Briefly, this test method has been designed to measure the fuel vapor pressure at a reference temperature of 37.8°C (100°F). A chilled sample (approximately 50 ml) was introduced into the bottom section of a two chamber vessel. The bottom (liquid) chamber and the top (vapor) chambers were connected and had a volumetric ratio of 1:4 (liquid:vapor). A pressure gauge was attached to the vapor chamber. Once filled with sample, the vessel was placed in a thermostatically controlled water bath set to 37.8°C. The vessel was removed from the bath every five minutes, inverted 5-10 times, and the vapor pressure was recorded. This was done until two sequential five minute recordings were within 0.1 psi, indicating that the sample was near equilibrium.

Speciation Analysis

Liquid composition analyses were performed using a gas chromatograph equipped with a flame ionization detector (GC/FID). Table 4.2 contains the list of target compounds quantified during this study. All target compounds were identified using GC/FID retention times established by analysis of various commercially-available

standards containing target compounds listed in Table 4.2 and quantified through use of one 5-point external standard calibration curve.

Target compound standards and sample composition analyses were performed by injection of a known amount of liquid gasoline, e.g., 1 μL, into a clean 125 mL glass sample bulb. After sufficient time had elapsed, allowing for complete evaporation of a sample, a solid-phase microextraction (SPME) fiber coated with polydimethylsiloxane (PDMS) was inserted into the sample bulb and exposed to the vaporized sample for 25 minutes. The fiber was then retracted, removed from the sampling bulb, and immediately analyzed by GC/FID.

Table 4.2. List of Target Compounds.

Compound	Chemical Abstract Number (CAS#)
Benzene	71-43-2
Biphenyl	92-52-4
Butane	106-97-8
Cis-2-Pentene	646-04-8
Cyclopentane	287-92-3
Cresol (o)[2]	95-48-7
Cresol (m)[2]	108-39-4
Cresol (p)[2]	106-44-5
Cumene	98-82-8
Decane	124-18-5
Dodecane	112-40-3
Ethylbenzene	100-41-4
Heptane	142-82-5
Hexane	110-54-3
Pentane	109-66-0
Methylcyclopentane	96-37-7
Methyl-tert-butyl ether	1634-04-4
Naphthalene	91-20-3
Nonane	111-84-2
Octane	111-65-9
Propane	74-98-6
Phenol	108-95-2
Styrene	100-42-5
Tetradecane	629-59-4
Toluene	108-88-3
Trans-2-pentene	627-20-3
Tridecane	629-50-5
Undecane	1120-21-4
Xylene (o)	95-47-6
Xylene (m)	108-38-3
Xylene (p)	106-42-3
1-Pentene	109-67-1
1,3,5-Trimethylbenzene	108-67-8
2,2,4 Trimethylpentane	540-84-1
2-Methyl-1-butene	563-46-2
2-Methyl-2-butene	513-35-9
2,2-Dimethylbutane	75-83-2
2,4-Dimethylpentane	108-08-7
2 –Methylpropane	75-28-5
2-Methylbutane	78-78-4
2-Methylpentane	107-83-5
3-Methlypentane	96-14-0

The GC/FID (Hewlett-Packard model 5870A) was equipped with a Hewlett-Packard PONA column (50 m, 0.2 mm i.d., 0.50 μm film thickness) and was operated with the following system parameters; injector temperature of 220 °C; initial oven temperature equal to 30 °C, hold for 7 min, ramp at 3 °C/min to 185 °C, hold for 5 min., ramp at 20 °C/min to 275 °C; detector temperature of 300 °C. The total run time was 68.2 minutes.

Sample Collection: Vapor

A special sampling apparatus (refueling sampler) was developed specifically for this research and was attached to the vehicle prior to refueling. The refueling sampler, as depicted in Figure 4.1, consisted of two concentric cylinders and was designed to allow for the capture of all fuel tank vapors displaced during refueling. The apparatus was connected to the vehicle fill-pipe using a screw-clamp, thus providing an air-tight seal at the fill-pipe connection. Gasoline was dispensed into the fuel tank after insertion of the fuel nozzle into the inside cylinder, which extended approximately four inches into the vehicle fill-pipe. Vapors displaced by dispensed gasoline were routed through the outside cylinder and exhausted via the exhaust chimney.

In preparation for vapor sample collection, a 1-liter glass bulb was evacuated to 15-inches mercury (Hg) vacuum. The bulb was attached to the sample line and opened, drawing 500 mL of headspace vapor into the sample bulb. This procedure served to purge the sample line of ambient air and replace it with headspace vapor. Vapor samples were collected immediately after completion of sample line "purge and fill." Vapor samples

were collected by attachment of partially evacuated 125 mL glass sample bulbs (3" Hg vacuum) to the sampling port. When evacuated to 3" Hg vacuum, a total of 12.5 mL of vapor entered the bulb resulting in a 10-fold dilution of the "stock" vapor exiting the fuel tank. Once filled, the sample bulb stopcock was closed and removed from the sampling line. One to two vapor samples were collected during each refueling experiment.

In addition to the refueling vapor samples, fuel tank headspace samples were also collected prior to refueling in order to allow for a comparison of pre-fill and refueling vapor composition. Fuel tank headspace samples were collected in a manner similar to the protocol described above for refueling samples. The only exception was that prior to attachment of the sampling apparatus to the fill-pipe a sample line was inserted approximately 12 inches into the fill-pipe. After insertion, the line was purged and a sample was collected as previously described, i.e., by use of an evacuated glass sampling bulb.

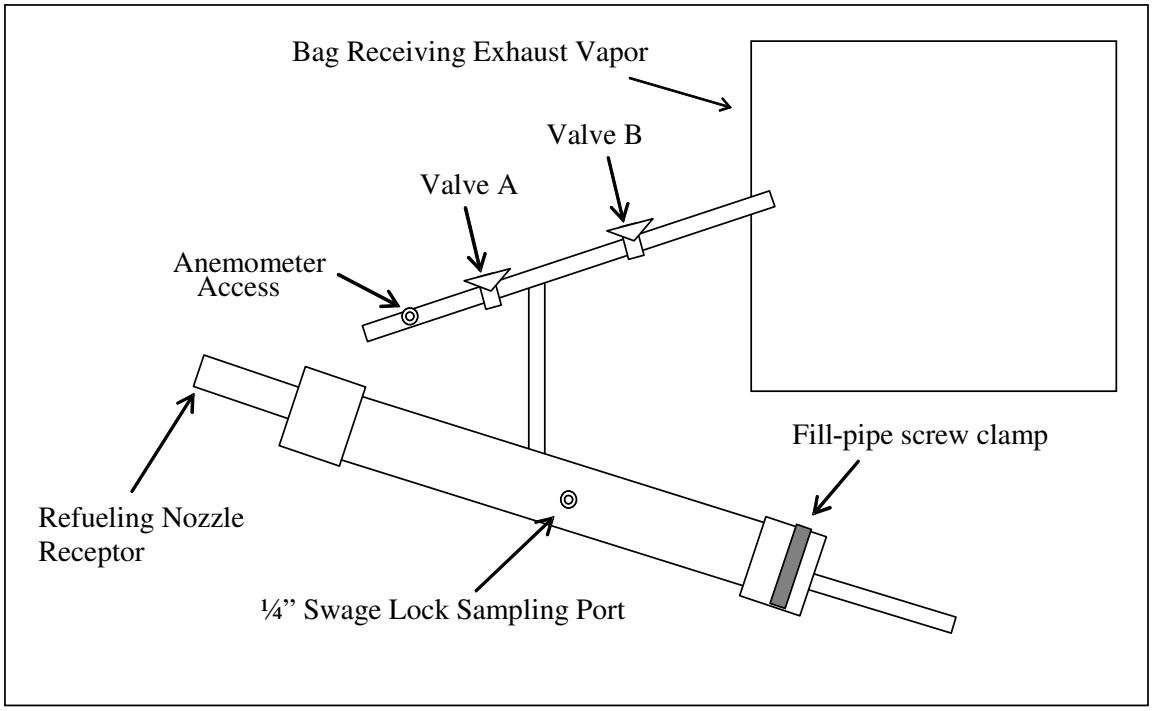

Figure 4.1. Schematic of Refueling Sampler Apparatus.

Vapor Flow Rate Measurement

Vapor flow rates were determined by two methods. The first utilized an existing algorithm developed to quantify the volume of vapor generated as a ratio of gasoline dispensed, i.e., volume vapor displaced/volume of gasoline dispensed. Specifically, volumetric flow rates were estimated for all experiments using Equation 3-3.

The second method was applied to experiments 7 through 12 and involved the capture of all displaced vapor during discharge of a known quantity of gasoline. To capture displaced vapors, valves A and B on the sampling apparatus (Figure 4.1) were positioned to direct all vapor into an empty air-tight sample bag. After dispensing a known volume of gasoline as indicated on the pump meter, both valves were repositioned

to direct vapor away from the bag and out the exhaust chimney. Valve B, which was in a closed position, and the filled sample bag were then removed from the sampling apparatus and immediately submerged in a small reservoir containing water at ambient temperature. After waiting several seconds to allow for surface agitation to subside, the water level was recorded on the inside of the reservoir. In addition, the water level associated with displacement caused by submerging an empty sampling bag and valve apparatus was recorded. Displaced vapor volumes were obtained by measuring the amount of water required to fill the reservoir from the empty-bag mark to the filled-bag mark. Vapor volume (liters) was then divided by volume of gasoline dispensed (gallons) resulting in a vapor flow rate expressed as liters of vapor/gallon of gasoline dispensed. During all experiments there was little, if any, difference in temperature between displaced vapor temperature and water, e.g., $\pm$ 3°C. Thus, it was assumed that vapor volume changes induced by heat transfer during bag submergence were insignificant.

Sample Analysis

Vapor sample analyses were performed by insertion of an SPME fiber into the glass sampling bulb and exposure of the fiber to the vapor sample for 25 minutes. The fiber was then retracted, removed from the bulb, and immediately analyzed by GC/FID as described previously under Speciation Analysis.

4.2. Evaporative Emissions Testing

The USEPA has developed a Federal Test Procedure for performing evaporative emissions testing. For a detailed description of the testing requirements the reader is referred to the Code of Federal Regulations §86.113-96 and §86.117-96 (United States Environmental Protection Agency, 1993). A core component of evaporative emissions testing is the use of an enclosure that is large enough to contain the entire test vehicle. Because the University of Texas at Austin does not have an enclosure of this type, completion of this testing was performed by Automotive Testing Laboratories, Inc. (ATL) located in Mesa, AZ. ATL has been involved with several studies related to exhaust and evaporative emissions testing of new and in-use vehicles.

Although ATL completed the testing, the testing conditions including vehicle emissions system, fuel and environmental conditions were selected by the author for this dissertation. Although standard evaporative emissions testing requires the determination of total VOC emissions during each test, testing performed as part of this project included the additional requirement of VOC speciation. This was considered important for understanding the role that the different types of evaporative emissions might have in terms of ozone formation.

4.2.1. Testing Overview

A total of eight experiments were performed. Each experiment involved the following:

1. Drain test vehicle fuel tank and refill to 40% full with test fuel.

2. Condition test vehicle with the test fuel (dynamometer operation) to remove any residual non-test fuel and to ensure that test results were associated with test fuel only.

3. Complete running loss test.

4. Complete hot soak test.

5. Complete 24-hour diurnal test.

All testing was completed in a sealed enclosure designed specifically for evaporative emissions testing of motor vehicles. Following EPA's test procedures, total VOC emissions for each test were determined as the difference between total VOC initial and final concentrations multiplied by the enclosure volume.

Enclosure Volume

The enclosure volume was determined by injecting a known mass of propane into the enclosure, mixing the air contents of the enclosure for at least five minutes and then measuring the concentration. Enclosure volume was quantified by dividing the mass injected by the concentration measured. This was then compared to volume quantified by multiplication of enclosure length, width and height measurements. The value to be used for volume based on this comparative method was considered acceptable when the two methods were within $\pm$2 %.

Total VOC Concentration

Total VOC concentrations were measured within the enclosure through the use of an on-line hydrocarbon FID analyzer calibrated against propane at the beginning and completion of each test.

VOC Speciation

Speciation profiles for each evaporative emissions test were determined as the difference between final and initial concentrations. Bag samples were taken and the beginning and end of each test and analyzed by a Varian Model 3400 GC-FID which utilized a 60 meter x 0.32 mm ID fused silica capillary column, thus providing compound identification and quantification.

4.2.2. Running Loss Test

For the running loss test, vehicles were pushed into an enclosure, the enclosure was sealed and then the vehicle was started and driven on a dynamometer for a defined period of time and speeds. Motor vehicle exhaust was routed outside of the enclosure using an exhaust hose to ensure that only evaporative emissions associated with the running losses were captured within the enclosure.

The driving program used for the running losses testing consisted of two different EPA driving patterns or cycles, the Urban Dynamometer Driving Schedule (UDDS) and the New York City Cycle (NYCC). The UDDS represents a total of 7.5 miles distance at an average speed of 19.6 miles/hr and has a test duration of approximately 23 minutes.

The NYCC is 1.18 miles in length, averages 7.1 miles/hr and has a duration of approximately 10 minutes. The entire driving cycle sequence used during the running loss test consisted of the following:

1. One UDDS
2. 2 minute vehicle idle
3. NYCC
4. NYCC
5. 2 minute vehicle idle
6. One UDDS
7. 2 minute vehicle idle

As a result of this sequence, the running loss test lasted a total of 72 minutes during which a total of 17.36 miles were simulated.

During the running loss test, the enclosure was maintained at a constant temperature to facilitate the determination of ambient temperatures on emissions. As a reference point, the USEPA has mandated 95º F as the standard test temperature which is employed in this study.

Through knowledge of the total distance traveled and the running loss emissions quantified during the test, an emission rate expressed in grams of VOC per mile traveled was determined.

4.2.3. Hot Soak Test

Immediately after completion of the running loss test, the vehicle was then pushed out of the running loss enclosure and placed within the hot soak enclosure. The enclosure was sealed and the evaporative emissions were measured over the next 60 minutes as the vehicle passively cooled down. Similar to the running loss test, the USEPA has mandated that an enclosure be maintained at a temperature of 95º F during the standard hot soak test, a condition employed in this research.

4.2.4. Diurnal Test

After completion of the hot soak test, each vehicle was allowed to cool down completely over a period ranging from 6 to 36 hours. This was done to ensure that the vehicle had stabilized after being operated during the running loss test. During the diurnal test, the temperature within the enclosure was cycled from a starting temperature to a maximum temperature and then back down to the initial temperature. The USEPA has mandated that for the standard 24 hour diurnal test the temperature profile range from 72 to 96º F, peaking at hour 9. Figure 4.2 contains the time-temperature profile specified by the USEPA (Coordinating Research Council 1998a) and employed in this study.

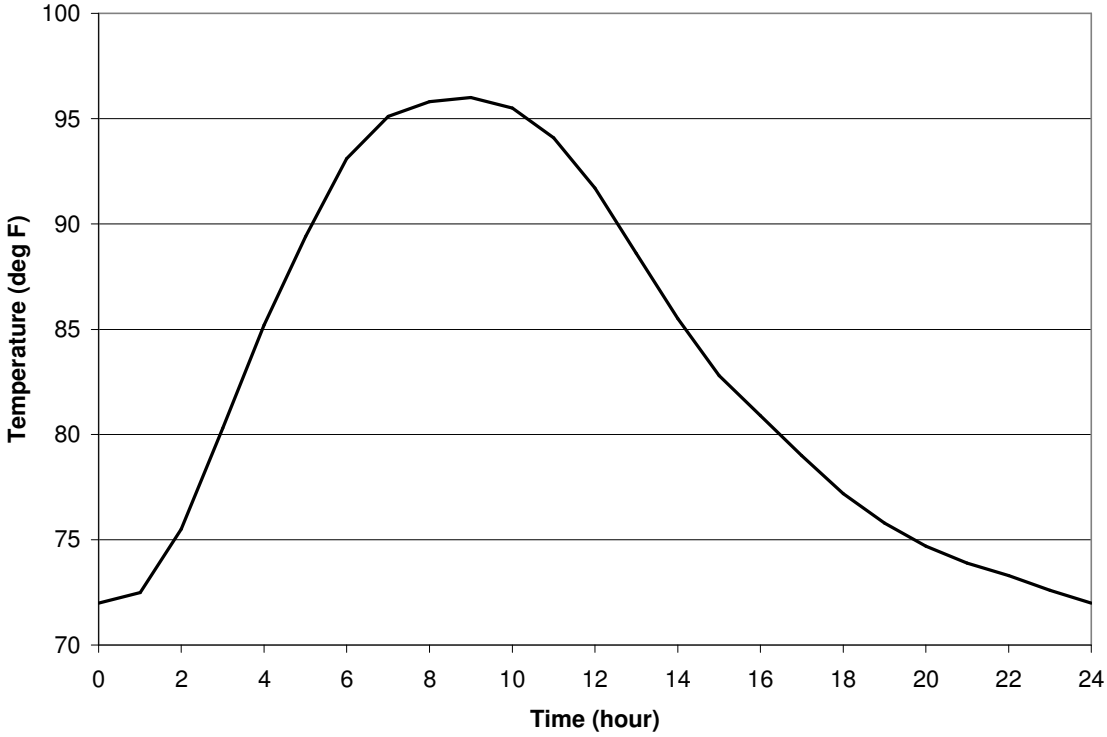

Figure 4.2. EPA's Standard 24-hour Diurnal Temperature Profile.

4.2.5. Experimental Plan Overview

Test Vehicles

Two different test vehicles were used during evaporative emissions testing. Prior to testing, each vehicle was inspected to ensure that all systems were operating properly. One vehicle was selected to represent older high mileage vehicles in the motor vehicle fleet, while the second vehicle was selected to represent a newer vehicle with moderate mileage. Relevant information for each vehicle is provided in Table 4.3.

Table 4.3. Test Vehicle Summary.

	Vehicle A	Vehicle B
Model Year	1987	1995
Make/model	Buick LeSabre	Nissan Maxima
Mileage	106,783	32,255
Engine/fuel system	3.8 L., port-fuel injected	3.0 L., port-fuel injected
Fuel Tank size (gallons)	18.0	18.5

Test Vehicle Conditions

Each vehicle was used during four tests. Two tests were completed with the vehicle in an "as-received" condition in terms of the evaporative emissions control system. For the other two tests, the evaporative emissions control system was disabled to facilitate the assessment of evaporative emissions from vehicles that had emissions systems tampered with, removed, or simply non-functioning. The evaporative emissions control system on Vehicle A was disabled by disconnecting the vent line between the fuel tank and the evaporative emissions canister, thus resulting in all evaporative emissions generated from the fuel tank to be simply emitted. Vehicle B was disabled by blocking the canister purge line. This prevented the normal purging of the canister during vehicle operation which is required to maintain canister adsorptive capacity.

Test Fuels

Two different fuels were tested. One fuel was gasoline certified to meet the USEPA's federal test specifications (most notably having an RVP value between 8.7 – 9.2 psi) and required to be used during EPA standard evaporative emissions testing. The second fuel selected for use was obtained in Houston, Texas, and represented an ozone

season reformulated gasoline with a reduced RVP. The use of this second fuel was intended to allow for the assessment of fuel impacts on evaporative emissions.

Environmental Conditions

Two sets of temperatures were used during the testing. Four experiments utilized one set of temperature conditions specified for use in the USEPA's federal test procedure, i.e., running loss and hot soak temperature of 95 ºF and diurnal profile of 72-96 ºF. The second set of temperatures was selected to be representative of conditions encountered in Texas during the summer season, i.e., running loss and hot soak temperature of 105 ºF and diurnal profile of 72-105 ºF. Although these temperatures are not expected to be encountered on a daily basis in Texas during the summer ozone season, it is a common occurrence to have daily maximum temperatures in excess of 95 ºF. Therefore, it was considered important to have an improved understanding of the impact that these higher temperatures might have on evaporative emissions.

A summary of the experimental program is provided in Table 4.4.

Table 4.4. Experimental Program for Determination of Evaporative Emissions..

Experiment No.	Fuel type	Temperature	Vehicle	Emissions Level
1[1]	Federal[2]	Federal[4]	A[6]	Regular[10]
2	Federal	Texas[5]	A	Regular
3	Federal	Federal	A*[7]	High[11]
4	Federal	Texas	A*	High
5	Federal	Federal	B[8]	Regular
6	Texas[3]	Federal	B	Regular
7	Texas	Federal	B*[9]	High
8	Texas	Texas	B*	High

1. Each experiment consisted of a running loss, hot soak and 24-hour diurnal evaporative emissions test.
2. Federal gasoline refers to gasoline certified to meet federal test specifications.
3. Texas gasoline used in testing was obtained from Houston during the 1999 summer ozone season and was intended to represent summertime reformulated gasoline available in the Houston ozone nonattainment area.
4. Federal temperatures used were:
   hot soak and running loss test temperatures: 95 °F
   24-hour diurnal test temperature profile: 72 to 96 °F
5. Texas temperature used were:
   hot soak and running loss test temperatures: 105 °F
   24-hour diurnal test temperature profile: 72 to 105 °F
6. Vehicle A was a 3.8 L, port-fuel injected 1987 Buick LeSabre equipped with an 18.0 gallon capacity fuel tank. At testing its odometer had 106,783 miles recorded.
7. A* indicates a disabled evaporative emissions control system status for Vehicle A.
8. Vehicle B was a 3.0 L, port-fuel injected 1995 Nissan Maxima equipped with an 18.5 gallon capacity fuel tank. At testing the odometer had 32,255 miles recorded.
9. B* indicates a disabled evaporative emissions control system status for Vehicle B.
10. Regular emission levels were associated with each vehicle during testing in their "as-received" or untampered condition.
11. High emission levels were associated with each vehicle in their "disabled" condition.

5. EXPERIMENTAL RESULTS

Results of refueling and evaporative emissions experiments are presented in Sections 5.1 and 5.2, respectively.

5.1. Uncontrolled Refueling Emissions

This section includes results related to refueling experiments. Measured and predicted vapor flow rates are presented, as are measured total and speciated vapor concentrations and emissions.

5.1.1. Vapor Flow Rates

Vapor flow rates determined using the two methods described in Section 4.1.1 are listed in Table 5-1. Algorithm-based (Equation 3-3) V/L ratios ranged from 3.0 to 3.8 liters of vapor/gallon of gasoline dispensed (L_{vap}/gal), with a mean and standard deviation of 3.5 L_{vap}/gal and 0.25 L_{vap}/gal, respectively. Bag-based volumetric flow rates ranged from 5.2 to 6.6 L_{vap}/gal with a mean and standard deviation of 5.5 L_{vap}/gal and 0.84 L_{vap}/gal, respectively. A hypothesis test on equality of means indicated that the measured (bag-based) vapor flow rate was significantly greater than the algorithm based value with a level of confidence of 95% ($\alpha = 0.05$).

Measured/estimated flow rate ratios are listed in Table 5-2. For all six experiments in which the bag method was used, the measured flow rates were higher than those estimated using Equation 4-1. The bag/algorithm method ratios ranged from 1.27 to 1.84 during experiments 7 through 12 with a mean value of 1.52.

Vapor flow rates for experiments 1 through 6 were calculated using flow rates obtained from the estimation algorithm and a correction factor of 1.52, which

corresponded to the mean bag/algorithm ratio. Flow rates used for all subsequent analyses are presented in Table 5-3.

Table 5-1. Algorithm- and Bag- Based Vapor Flow Rates.

	Algorithm Method					Bag Method
Experiment	T_d (°F)	T_t (°F)	RVP (psi)	V/L[1]	V/L[2]	V/L[3]
1	63	75	12.7	0.80	3.03	-
2	63	75	12.7	0.80	3.03	-
3	73.8	78.8	11.0	0.92	3.48	-
4	73.8	78.8	11.0	0.92	3.48	-
5	73.4	80	11.4	0.89	3.37	-
6	73.4	80	11.4	0.89	3.37	-
7	91	93.8	9.6	0.95	3.60	4.56
8	91.1	92.9	9.3	0.97	3.67	4.66
9	85.7	92.4	8.4	0.89	3.37	6.21
10	85.7	87.0	9.5	0.98	3.71	5.82
11	91.1	93.8	10.0	0.97	3.67	6.60
12	85.7	84.8	8.15	1.01	3.82	5.15

1. V/L = volume vapor displaced/volume gasoline dispensed in gallons vapor / gallon gasoline.
2. V/L = volume vapor displaced/volume gasoline dispensed in liters vapor / gallon gasoline and obtained by multiplying gallon vapor/gallon gasoline by 3.785 L/gal.
3. V/L = volume vapor displaced/volume gasoline dispensed in liters vapor / gallon gasoline.

Table 5-2. Measured vs Estimated Flow Rate Ratios.

Experiment	Bag/Algorithm ratio
1	-
2	-
3	-
4	-
5	-
6	-
7	1.27
8	1.27
9	1.84
10	1.57
11	1.80
12	1.35
Average	1.52
Standard deviation	0.26
Relative standard deviation	17.1%

Table 5-3. Displaced Vapor Flow Rates.

Experiment	Flow rate V/L (L vapor/gallon gasoline)
1	4.61[1]
2	4.61[1]
3	5.29[1]
4	5.29[1]
5	5.12[1]
6	5.12[1]
7	4.56
8	4.66
9	6.21
10	5.82
11	6.60
12	5.15

1. Flow rates obtained by multiplying algorithm-based flow rates in Table 5-1 by 1.52.

5.1.2. Total VOC Concentrations

Total VOCs present in the headspace of fuel tanks prior to refueling (pre-fill) and average refueling total VOC concentrations for each experiment are listed in Table 5-4. Pre-fill total VOC concentrations ranged from 0.01 to 1.53g/L with a mean and standard deviation of 0.65 g/L and 0.47 g/L, respectively. Refueling total VOC concentrations ranged from 1.04 to 1.66 g/L and had mean and standard deviations of 1.33 g/L and 0.26 g/L, respectively. A hypothesis test on equality of means indicated that the refueling VOC concentration was significantly greater than the prefill concentration with a level of confidence of 95% ($\alpha = 0.05$).

The fact that mean VOC concentrations during refueling were significantly higher than pre-fill headspace concentrations suggests that significant mass transfer occurs from fresh (dispensed) gasoline during refueling. However, the ratio of refueling to pre-fill total VOC concentrations varied considerably between events and precludes any attempt to determine the relative contribution of aged and fresh gasoline vapors to total VOC emissions during refueling. Factors which might affect such contributions include the age of pre-fill vapors, temperatures of aged and fresh gasolines, volume of gasoline remaining in the fuel tank prior to filling, and fill rate. The latter two factors should have a significant impact on degree of splashing/mixing within the tank during refueling and, hence, on gas-liquid mass transfer.

Table 5-4. Pre-fill and Average Refueling VOC Concentrations.

Experiment	Pre-fill VOC (g/L)[1]	Average Refueling VOC (g/L)
1	0.01	1.47
2	0.13	1.33
3	0.39	1.04
4	0.33	0.73
5	0.11	1.59
6	0.91	1.38
7	1.53	1.58
8	0.71	1.25
9	1.01	1.66
10	1.14	1.38
11	0.85	1.39
12	0.72	1.11

1. g/L refers to mass of total VOCs per volume of vapor (not volume of dispensed gasoline).

Refueling total VOC concentrations were also estimated for each experiment based on an assumption of vapor-liquid equilibrium (Raoult's law), the ideal gas law, dispensed gasoline RVP, dispensed liquid gasoline and tank headspace temperatures, and gasoline vapor molecular weight algorithms developed for AP-42 (Shedd, 1992). Measured and estimated VOC concentrations are presented in Figure 5-1. Estimated total VOC concentrations were calculated using dispensed gasoline and resident headspace temperatures in order to provide a range of potential values. The ratio of average measured to estimated VOC concentrations based on dispensed and tank headspace temperatures were 0.96 and 0.88, respectively. However, the measured minimum VOC concentration was approximately 50% of the estimated minimum VOC concentration. This result suggests that total VOC concentration during refueling may be more sensitive to system and environmental conditions than can be explained by an assumption of ideal

equilibrium conditions. In particular, some conditions may lead to mass transfer limitations which inhibit an approach to equilibrium.

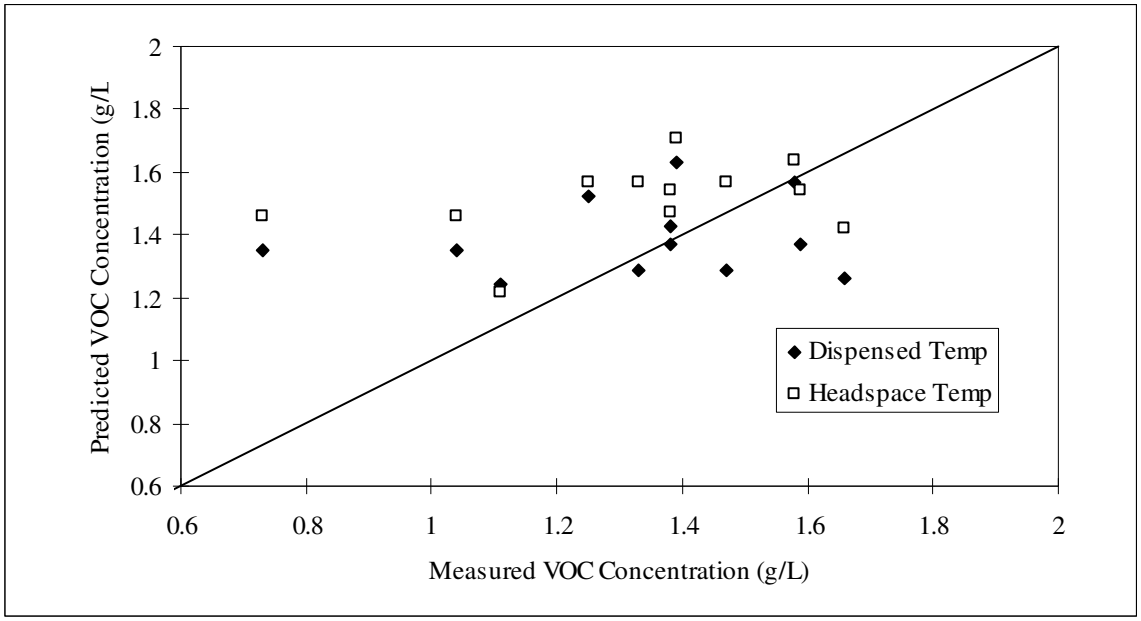

Figure 5-1. Predicted versus Measured Refueling Total VOC Concentrations.

5.1.3. Speciated VOC Concentrations

Speciated concentrations were determined for all target VOCs (see Table 4-2 for a list of target compounds) for each experiment and are provided in Appendix A, Tables A-1 through A-12. Concentrations were determined prior to filling (pre-fill), i.e., aged vapor, and during refueling. An average VOC concentration during refueling was also determined for each experiment. In addition, average refueling gasoline vapor compositions for the summer and winter seasons were determined and are included in Appendix A (Table A-13 and A-14). Target compounds comprised at least 88% of total

VOCs, with the five most abundant compounds (2-methylbutane, butane, pentane, 2-methylpentane and 2-methyl-2-butene) accounting for more than 69% of total VOC mass.

For urban areas required to complete photochemical modeling, emission inventories and speciation profiles are required. For areas that have not developed local speciation profiles, the use of speciation profiles developed elsewhere is often necessary. The following analyses have been completed to determine potential differences between use of local speciated profiles and other available profiles.

The average summer vapor profile obtained during this study was compared to the Southern Oxidant Study vapor speciation profile (SOSVAP) and the CARB summer vapor speciation profile (VGS710) in order to assess the validity of the use of either of these profiles for studies in which actual vapor speciation data are not available. The SOSVAP and VGS710 profiles were obtained from the VOC Source Apportionment Coastal Oxidant Assessment For Southeast Texas Study (Fujita *et al*., 1995b), and are included in Appendix A (Table A-15). Results of this comparison are presented in Figure 5-2a through 5-2f, and are tabulated in Appendix A (Table A-16). The comparison was limited to compounds identified in both profiles.

Of the 25 compounds included in this comparison, five compounds had absolute percent by weight differences greater than 1% (SOSVAP or CARB relative to measured values). These were: iso-butane, butane, iso-pentane, pentane, and 2-methylpentane. The most noticeable difference was for butane, which comprised <10% of the vapor composition by weight in Austin in contrast to between 20-30% by weight for the SOSVAP and CARB profiles. For all five compounds the absolute difference between

the CARB profile and measured vapor concentrations were larger than the difference between the SOSVAP and Austin summer vapor profiles.

Twelve compounds had absolute percent by weight differences of less than 0.5%. These were: cyclopentane, methylcyclopentane, benzene, heptane, octane, ethylbenzene, m,p-xylene, styrene, o-xylene, nonane, cumene, and 1,3,5- trimethylbenzene. For the eight remaining compounds, the absolute difference between the CARB profile and Austin average summer vapor profile were larger than the difference between the SOSVAP and Austin summer vapor profiles with the exception of toluene.

Normalized standard errors were calculated for the SOSVAP-Austin average summer profile and CARB-Austin average summer vapor profile comparisons. Normalized standard error values were obtained using the following equation:

$$S_e = \frac{S}{\sqrt{n}} \tag{5-1}$$

$$S = \sqrt{\frac{\sum\left(\frac{y_i - y}{y}\right)^2}{n-1}} \tag{5-2}$$

where:

S_e = normalized standard error;

S = normalized standard deviation;

n = total number of compounds;

y_i = compound$_i$ profile value; and

y = compound$_i$ measured value.

Normalized standard error values for the SOSVAP-Austin and CARB-Austin average summer vapor profile comparisons were 0.157 and 0.342, respectively. Thus, based on this evaluation, the SOSVAP profile would be a better profile than the CARB profile to use in the Austin area during summer (if an actual profile was not available).

Another potential vapor speciation profile generation scenario involves the estimation of vapor profiles based on available liquid speciation profiles. For this evaluation, vapor concentrations were estimated based on liquid composition for the same compounds contained in the SOSVAP and CARB comparisons. Predicted vapor concentrations were calculated using liquid RVP and composition data, dispensed gasoline temperature, and Raoult's Law. Predicted versus measured concentrations for Experiments 7 through 12 (corresponding to summer experiments) are presented in Figure 5-3. Over all six summer experiments the average predicted/measured concentration ratio was 0.83.

To assess the validity of predicting vapor compositions based on liquid composition data, an average summer vapor profile was generated using the six summer experiments. This profile is included in Appendix A (Table A-16). The average summer vapor profile predicted using liquid composition data was generally more accurate than either the SOSVAP or CARB profiles, and had a normalized standard error of only 0.065. It should be noted that the average vapor profile predicted using the liquid composition

data was calculated using dispensed gasoline temperature. The use of higher temperatures, e.g., tank headspace vapor temperature (T_v), may be more realistic given that initial fuel tank temperatures. It is expected that the actual temperature that should be used for vapor composition predictions is between T_d and T_v.

A comparison of measured and predicted (based on liquid composition) vapor speciation concentrations was performed for eight compounds. Compounds included in this comparison were: methyl-tert butyl ether (MTBE), hexane, benzene, 2,2,4-trimethylpentane (2,2,4-TMP), toluene, ethylbenzene (Ethylbenz), m,p-xylene (m,p-Xyl), and o-xylene (o-Xyl). Predicted concentrations were calculated assuming vapor-liquid gasoline equilibrium, use of the ideal-gas law, dispensed liquid gasoline composition and temperature, and RVP of the dispensed gasoline.

Measured/predicted concentration averages, standard deviations, and relative standard deviations are listed in Tables 5-5 and 5-6 by compound and experiment, respectively. In addition, the average measured/predicted concentration ratio and standard deviation for each VOC over all 12 experiments is plotted in Figure 5-4.

Based on these results, it is evident that there is substantial variation in the comparative results between measured and predicted vapor concentrations. This is most likely due to experimental conditions that cause the assumption of vapor-liquid equilibrium to be incorrect, e.g., splashing/mixing during refueling that impacts gas-liquid mass transfer. Further, the use of the dispensed temperature would tend to minimize the predicted vapor concentrations. This may help to partially explain the fact that three VOCs (Benzene, Toluene, and m,p-Xylenes) had average measured/predicted concentration ratios above 1.

Use of a higher temperature that might be closer to the actual liquid temperature within the tank would increase the predicted concentration and thereby lowering the measured/predicted ratio.

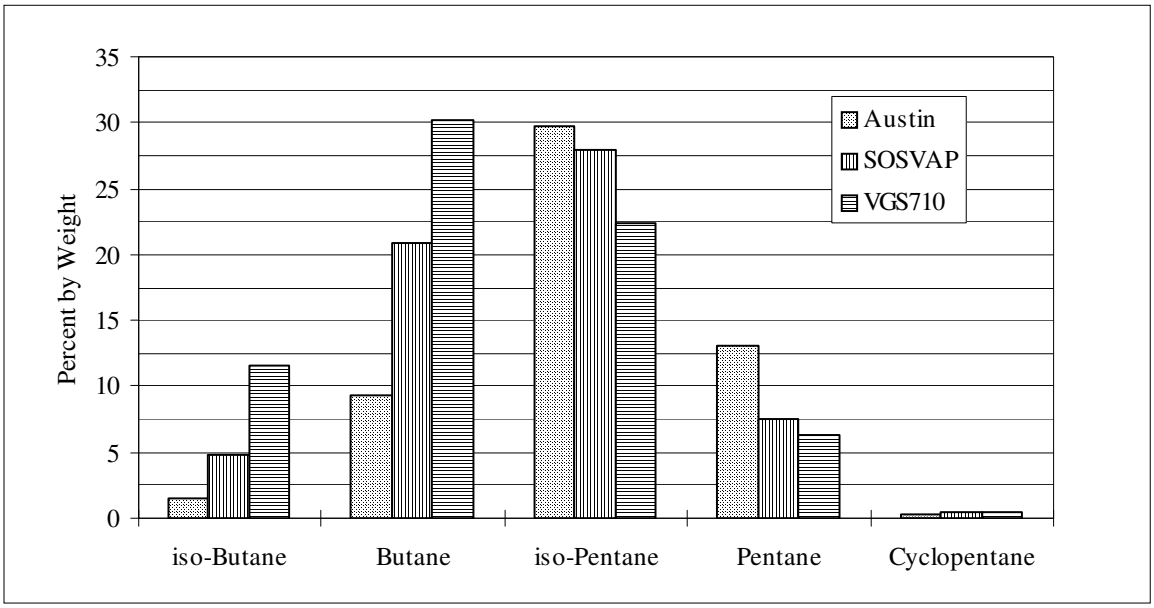

Figure 5-2a. Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (Butanes and Pentanes).

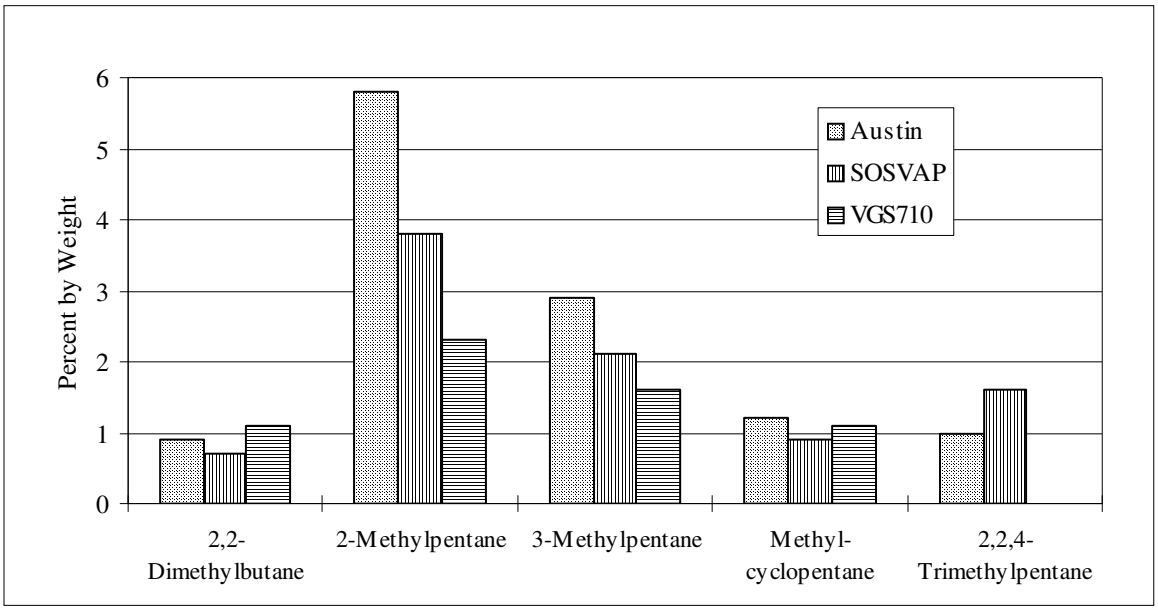

Figure 5-2b Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (Methylated Butanes and Pentanes).

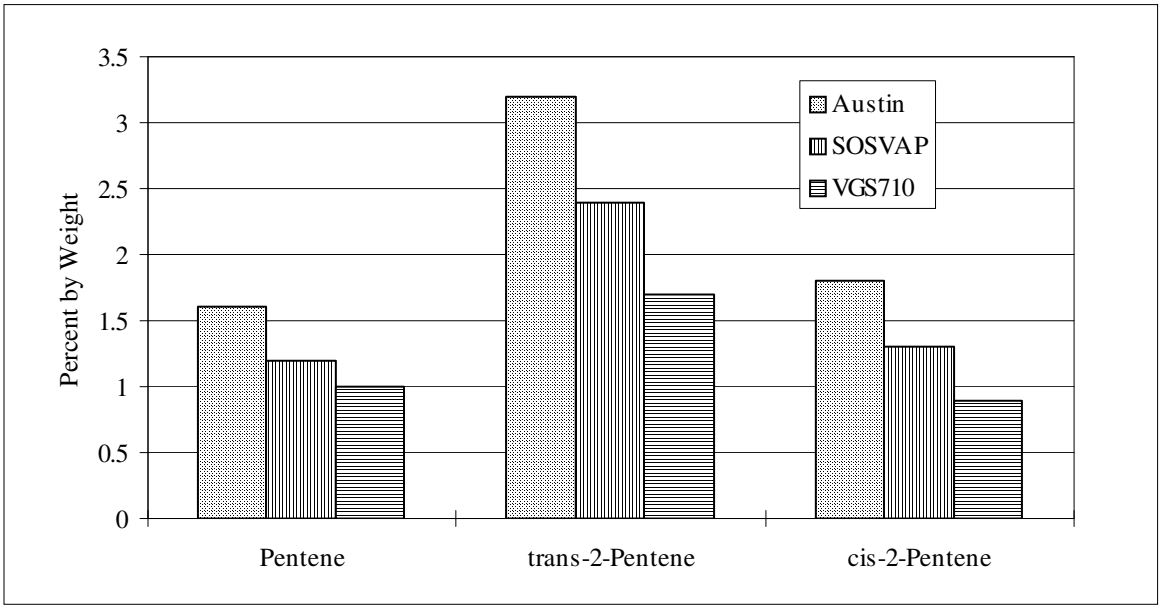

Figure 5-2c. Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (Pentenes).

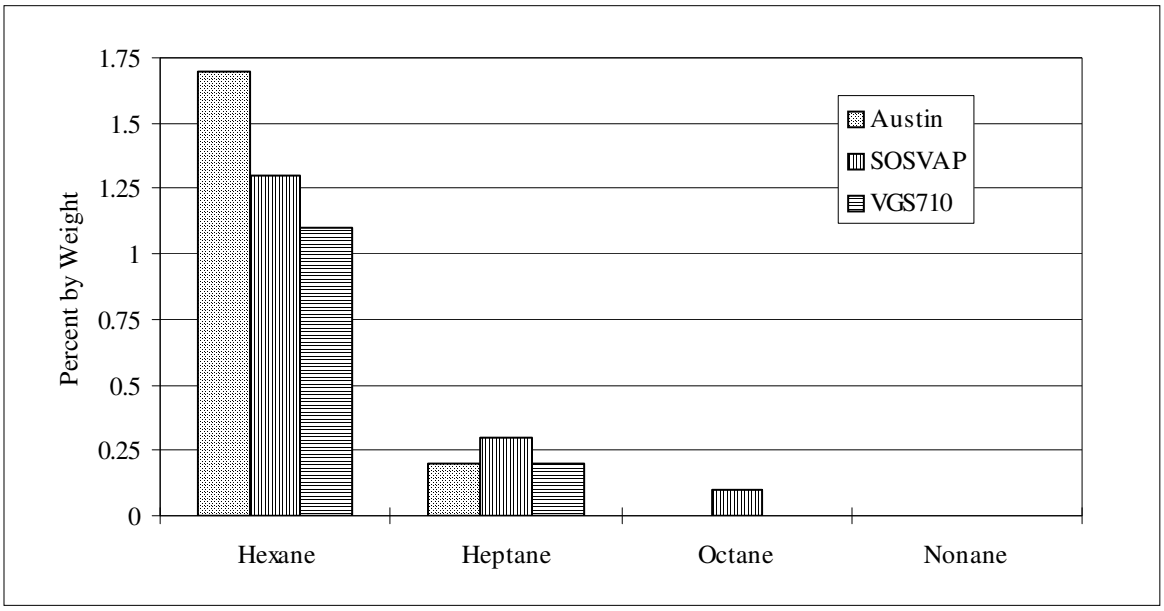

Figure 5-2d. Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (Higher alkanes).

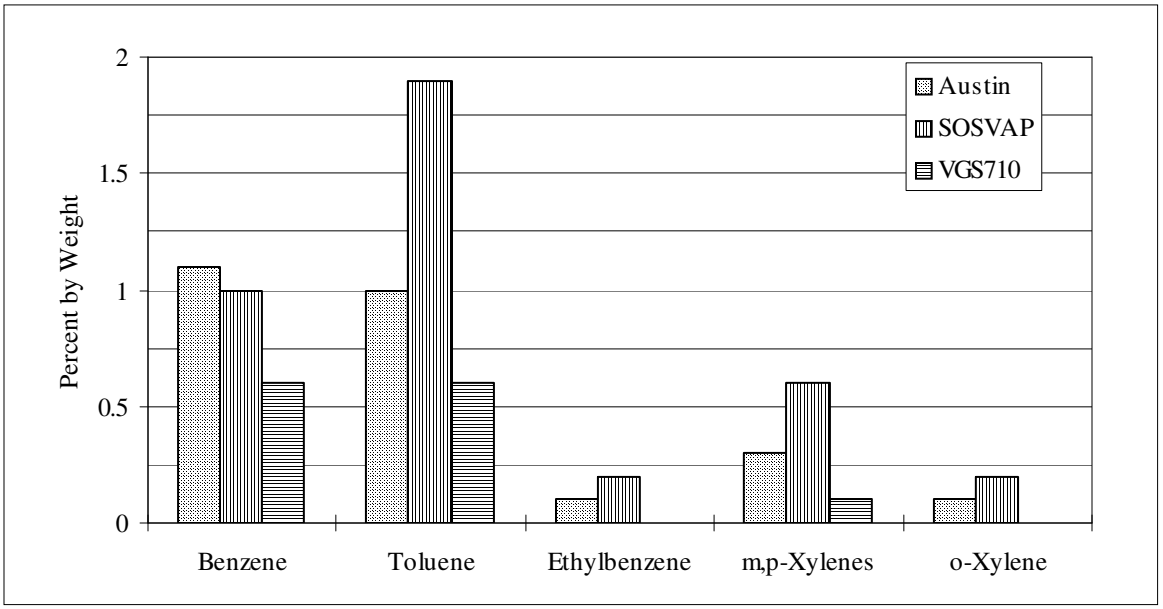

Figure 5-2e. Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (BTEX).

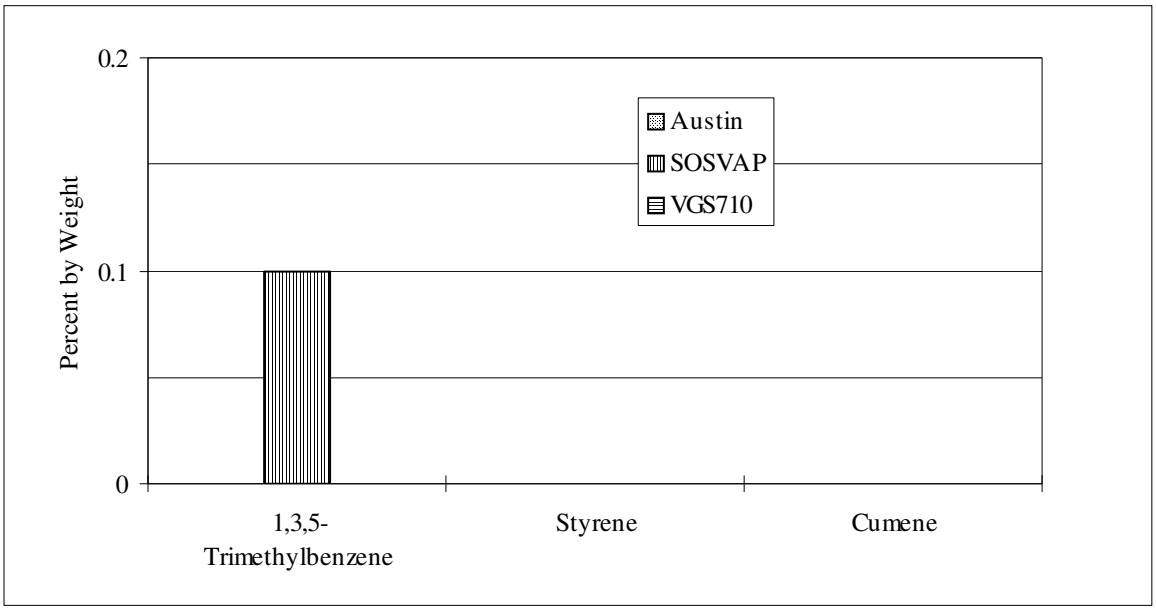

Figure 5-2f. Austin, Southern Oxidant Study, and CARB Gasoline Vapor Summer-Blend Speciation Profiles (Others).

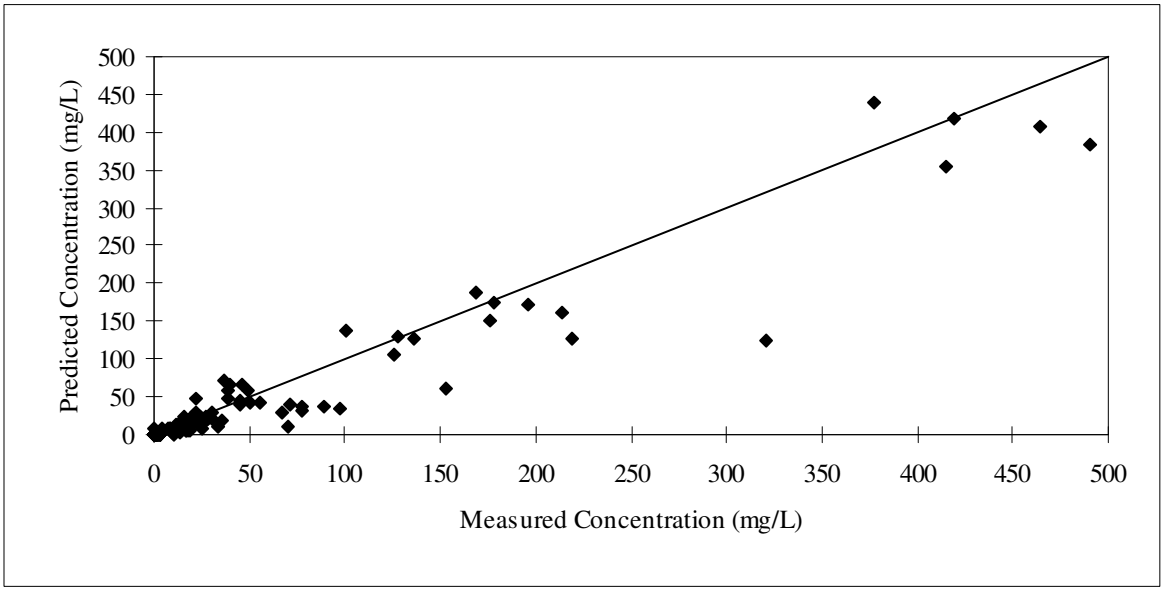

Figure 5-3. Predicted versus Measured Vapor Concentrations: Experiments 7 to 12.

Table 5-5. Measured/Predicted Concentration Ratio (by compound).

	Measured/Predicted Concentration		
Compound	Average (n = 12)	Standard Deviation	Relative Standard[1] Deviation (%)
MTBE	0.97	0.37	37.7
Hexane	0.93	0.36	38.7
Benzene	1.14	0.51	44.6
2,2,4-Trimethylpentane	0.88	0.53	60.3
Toluene	1.04	0.53	51.0
Ethylbenzene	0.88	0.59	67.0
m,p-Xylenes	1.34	0.82	61.7
o-Xylene	0.96	0.69	71.5

1. (standard deviation/average)*100

Table 5-6. Measured/Predicted Concentration Ratio (by experiment).

	Measured/Predicted Concentration		
Experiment	Average (n = 8)	Standard Deviation	Relative Standard[1] Deviation (%)
1	1.24	0.42	34.2
2	1.35	0.47	34.9
3	0.61	0.21	34.2
4	0.37	0.12	32.9
5	0.48	0.30	62.3
6	0.26	0.07	28.9
7	1.05	0.15	13.9
8	1.01	0.1	9.5
9	2.07	0.56	27.3
10	1.3	0.13	10.3
11	1.27	0.13	10.4
12	1.19	0.32	27.1

1. (standard deviation/average)*100

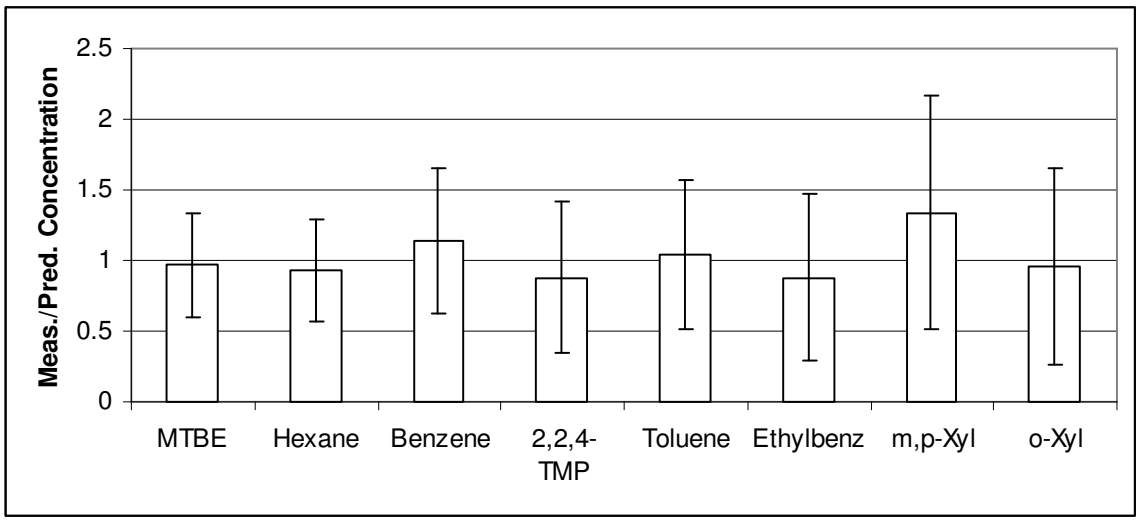

Figure 5-4. Average Speciated Compound Measured vs. Predicted Concentration Comparison.

5.1.4. Total VOC Emission Rates

Total VOC emissions (expressed as gram VOC/gallon gasoline dispensed) were obtained for each vehicle refueling experiment by multiplying vapor volumetric flow rate (liters vapor/gallon gasoline dispensed) and total VOC concentration (gram VOC/liter vapor). Vapor flow rates, total VOC concentrations, and total VOC emissions for each experiment are listed in Table 5-7. The range of total VOC emission rates over all experiments was 3.9 to 10.4 g VOC/gallon gasoline dispensed. The mean and standard deviations were 7.0 g VOC/gallon and 1.8 g VOC/gallon, respectively.

Table 5-7. Total VOC Emission Rates for Vehicle Refueling.

Experiment	Vapor Flow rate (L vapor/gallon gasoline)	Total VOC Concentration (g VOC/L vapor)	Total VOC Emissions (g VOC/gallon gasoline)
1	4.61	1.47	6.78
2	4.61	1.33	6.13
3	5.29	1.04	5.50
4	5.29	0.73	3.86
5	5.12	1.59	8.14
6	5.12	1.38	7.06
7	4.56	1.58	7.17
8	4.66	1.25	5.84
9	6.21	1.66	10.4
10	5.82	1.38	8.02
11	6.60	1.39	9.19
12	5.15	1.11	5.72

A common method used to estimate total VOC emissions during automobile refueling is based on the application of EPA's MOBILE model. The current version of this model is MOBILE6 which is an updated version of MOBILE5A (USEPA, 1994c). However, the code associated with refueling emissions has not been revised between the two models. Therefore, for the purpose of this dissertation, predicted results were obtained using MOBILE5A.

Model output is used to generate refueling emission factors that are used in conjunction with gasoline consumption rates to estimate total refueling emissions for a prescribed geographic area, e.g., county or larger airshed. Refueling emissions in MOBILE5a are estimated as the sum of spillage and displacement emissions. Spillage emissions are assumed to have a constant value of 0.31 g/gallon pumped, i.e., independent of fuel/ambient temperatures and fuel RVP. Displacement emissions (the

focus of this study) were estimated using Equation 3-4. Within MOBILE5a, fuel RVP is entered by the user. However, both the dispensed gasoline temperature (T_d) and the difference between dispensed and resident (in-fuel tank) gasoline temperatures (ΔT) are not user-prescribed. The MOBILE5a model includes an algorithm that relates the dispensed gasoline temperature to minimum and maximum ambient temperatures, and the temperature difference (ΔT) to the estimated value of T_d. The dispensed fuel temperature is limited to the range of 20 – 95 ºF while ΔT is set to be equal or less than 20 ºF.

A comparison between measured and predicted emission rates was performed. One algorithm selected for comparison is Equation 3-4, currently serving as the basis for refueling emissions calculated using AP-42.

The second algorithm used in the comparison was developed by Cingle and McClement (1988). This algorithm (Equation 3-7) was used in the On-board Refueling Vapor Recovery (ORVR) Standard Final Regulatory Impact Analysis (United States Environmental Protection Agency, 1994b) to determine baseline emissions.

Measured versus predicted emissions using the Rothman and Johnson (AP-42) and Cingle and McClement (ORVR) algorithms are plotted in Figure 5-5, and are also tabulated in Appendix A (Table A-17). Measured emissions either exceeded or were equal to predicted emissions using either algorithm in ten of the twelve experiments. Predicted emissions based on either algorithm ranged from 4.6 to 6.7 g VOC/gallon. Emissions derived from the AP-42 algorithm (Equation 5-3) were higher than ORVR emissions for ten of the twelve experiments. Overall measured/predicted average

emission ratios were 1.26 and 1.32 for AP-42 and ORVR, respectively. However, if the comparison is limited to experiments completed during the ozone season, i.e., Experiments 7 to 12, the measured/predicted emissions for AP-42 and ORVR increase to 1.28 and 1.39, respectively. Thus each algorithm may significantly underestimate VOC emissions during the ozone season.

The Texas Commission on Environmental Quality (TCEQ) relies on the MOBILE family of models (at present MOBILE6 which utilizes MOBILE5A refueling codes) to estimate refueling emissions of VOCs within specific airsheds. For example, average daily refueling losses in Austin for the 1997 ozone season were estimated to be 4.0 g/gal. This emission factor is based on an assumed RVP of 8.1 psi and minimum and maximum ambient temperatures of 73°F and 94°F, respectively. If spillage emissions are subtracted from the refueling emissions, displacement losses are estimated to be 3.7 g/gal.

Experiments 7 through 12 were completed in Austin during the 1997 summer ozone season. If values of T_d, T_t (or ΔT), and RVP measured during those experiments are substituted into Equations 5-3, displacement emissions are estimated to range from 4.9 to 6.7 g/gal, with an arithmetic mean of 6.1 g/gal (a factor of approximately 1.7 higher than the MOBILE5a 3.7 g/gal estimate). Measured emission rates for Experiments 7 through 12 ranged from 5.7 to 10.4 g/gal, with an arithmetic mean of 7.7 g/gal.

The difference between the TCEQ-estimated value of 3.7 g/gal and those based solely on Equation 5-3 (with measured input variables) and field measurements may be due to several factors. First, the predicted value was based on an RVP of 8.1 psi. Values

of RVP measured for each of the six summer monitoring events in Austin ranged from 8.2 to 10 psi with an arithmetic mean of 9.2 psi. To assess the impact of RVP on VOC emissions estimates, Equation 5-3 was used with an RVP of 8.1 psi. The average displacement loss decreased from 6.1 g/gal (using measured RVP) to 5.6 g/gal, a value that is still considerably higher than the MOBILE5a estimate. Thus, while differences in RVP can account for some differences in displacement emissions estimates between MOBILE5a and either Equation 5-3 (with measured input) or field measurements, values of dispensed and resident fuel temperatures must play a very important role.

The MOBILE5a estimate of 3.7 g/gal was determined as an average daily refueling loss based on minimum and maximum daily temperatures ranging from 73°F to 94°F. In fact, most of the field monitoring events completed for this study were at times when the ambient temperature approached or exceeded 90°F. When the MOBILE5a model is executed with an RVP = 8.1 psi and minimum and maximum temperatures fixed at 90°F, displacement losses are estimated to be 4.1 g/gal. While this value is closer to the mean values based on Equation 5-3 (with measured input) or field measurements, it is still considerably lower than (nearly a factor of 2) field measurements. This difference is great enough to warrant concern regarding existing emission inventories that utilize MOBILE5a for estimating refueling losses for light-duty gasoline vehicles and trucks, and to recommend future research to improve such estimates.

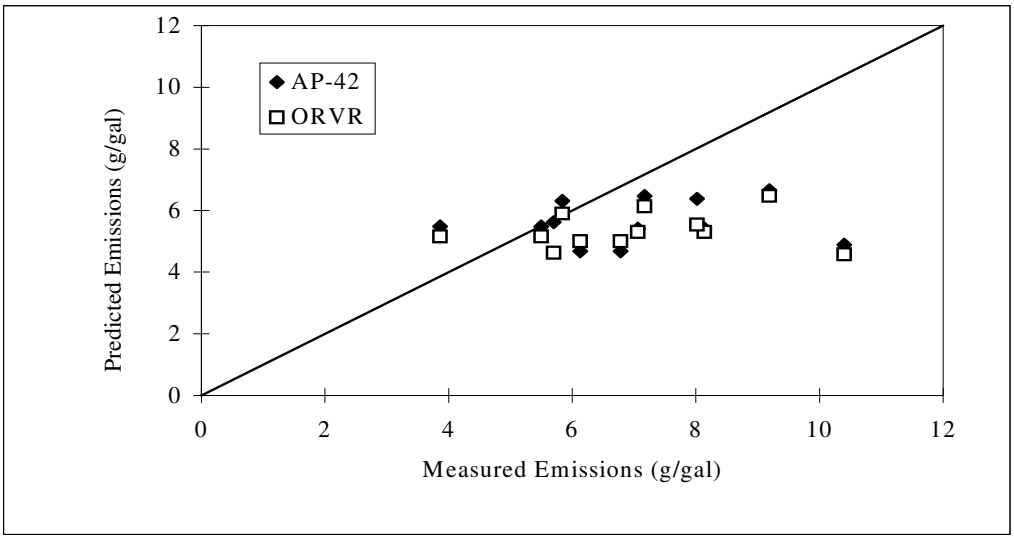

Figure 5-5. Predicted vs. Measured Refueling Emissions.

5.1.5. Speciated Compound Emissions

Speciated emissions were determined for all target compounds and individual experiments. Corresponding results are included in Appendix A (Tables A-1 through A-12). Emission rates (µg/gallon gasoline dispensed) were obtained by multiplying compound concentrations (µg/L vapor) by total vapor volumetric flow rate (L vapor/gallon gasoline dispensed). Averaging over all 12 experiments, butane and iso-pentane made up greater than 45% of total VOC emissions. Five compounds, including butane, iso-butane, iso-pentane, 2-methylpentane, and 2-methyl-2-butene comprised greater than 69% of total VOC emissions.

A comparison between measured and predicted summer season emission rates was performed. Predicted emissions were calculated using total VOC emission rates based on the MOBILE5a total VOC refueling estimate of 3.7 g/gal coupled with the

SOSVAP vapor speciation profile (Table A-16). Average measured emissions for individual compounds were obtained by using the average VOC refueling emissions value of 7.7 g/gal coupled with the average summer Austin vapor profile (Table A-16). Results are provided in Table 5-8 for all compounds with a measured concentration $\geq$ 1.0 percent.

A total of 14 compounds had individual average concentrations $\geq$ 1.0 percent. Within this subset, measured emissions exceeded predicted emissions for all but two compounds (butane and iso-butane). Measured/predicted ratios for the top 14 compounds ranged from 0.65 to 3.61, and averaged 2.29. For all compounds present in both profiles with non-zero concentrations, the measured/predicted ratio was 1.85.

Results of this comparison indicate that use of MOBILE5a-based total VOC emissions estimates coupled with existing gasoline vapor speciation profiles may lead to significant errors (underestimation) with respect to speciated compound emissions. Implications associated with these underestimations are discussed in the next chapter.

Table 5-8. Measured vs Predicted Summer Season Individual Compound Emissions.

Compound	Measured Conc. (%)[1]	Measured Emiss. (g/gal)[2]	Predicted Conc. (%)[3]	Predicted Emiss (g/gal)[4]	Emissions Meas/Pred
iso-Pentane	29.7	2.29	28	1.04	2.21
Pentane	13	1.00	7.5	0.28	3.61
Butane	9.3	0.72	20.9	0.77	0.93
2-Methylpentane	5.8	0.45	3.8	0.14	3.18
trans-2-Pentene	3.2	0.25	2.4	0.09	2.77
3-Methylpentane	2.9	0.22	2.1	0.08	2.87
cis-2-Pentene	1.8	0.14	1.3	0.05	2.88
Hexane	1.7	0.13	1.3	0.05	2.72
Pentene	1.6	0.12	1.2	0.04	2.77
iso-Butane	1.5	0.12	4.8	0.18	0.65
Methylcyclopentane	1.2	0.09	0.9	0.03	2.77
Benzene	1.1	0.08	1	0.04	2.29
2,2,4-TMP	1	0.08	1.6	0.06	1.30
Toluene	1	0.08	1.9	0.07	1.10
Total	74.8	5.76	78.7	2.91	

1. Summer average vapor concentration profile
2. Measured compound emission rates obtained by multiplying compound concentration by measured average refueling emission rate of 7.7 g/gal
3. SOSVAP vapor profile
4. Predicted compound emission rates obtained by multiplying compound concentration by MOBILE5a predicted summer average refueling emission rate of 3.7 g/gal

5.2 Evaporative Emissions Results

As discussed in Chapter 4, an evaporative emissions testing program was developed and completed as part of this research. The experimental plan is summarized in Table 4-4.

5.2.1 Total VOC Emissions Results

Evaporative emissions category-specific total VOC emissions measured during each experiment are provided in Table 5-9**.**

Table 5-9. Running Loss, Hot Soak and Diurnal Total VOC Emissions.

Experiment	Running Loss (g/mi)[1]	Hot Soak (g/test)[2]	Diurnal (g/test)[3]
1	2.66	2.26	26.47
2	18.37	53.20	37.68
3	14.92	6.71	28.04
4	28.14	26.93	41.58
5	7.13	3.69	13.32
6	0.26	0.29	2.59
7	7.97	3.95	18.80
8	14.78	4.64	26.97

1. Running loss emissions were calculated as the total mass measured in SHED divided by total dynamometer miles traveled.
2. Hot soak emissions were quantified at the end of the 1-hour hot soak test.
3. Diurnal emissions were quantified at the end of the 24-hour diurnal test.

As a result of the different fuel types, temperatures and vehicles used, the range of evaporative emissions measured was large. Running loss emissions ranged from 0.26 to 28.14 g/mi, a difference of greater than two orders of magnitude. Hot soak emissions had a maximum:minimum emissions ratio in excess of 180:1 (53.2 vs. 0.29 g/test). The diurnal emissions maximum:minimum ratio was 16:1, corresponding to values of 41.6 and 2.59 g/test, respectively. Experiment 6, which included the lower RVP fuel, lower temperatures and the newer vehicle had the lowest emissions for all three evaporative

emissions categories. Experiments 2 and 4 which utilized the higher RVP federal fuel, higher temperatures, and the older vehicle had the highest emissions.

The experimental plan facilitated an investigation of the effects of three individual parameters on evaporative emissions. These were:

- fuel type, i.e., Texas summer RFG vs Federal test fuel
- environmental conditions, i.e., Texas-specific vs Federal test conditions
- evaporative system controls, i.e., disabled vs "as-received"

Table 5-10 includes summary information of these parameter-specific comparisons.

Table 5-10. Effects of Temperature, Fuel type and Emissions Control Systems on Evaporative Emissions.

Parameter	Experiments	Emissions Ratio Metric	Emissions Ratio Results		
			Running Loss	Hot Soak	Diurnal
Fuel[1]	5 vs 6	Fed/TX[4]	27.4	12.7	5.1
Temp[2]	1 vs 2	TX/Fed[5]	6.9	23.5	1.4
	3 vs 4	TX/Fed	1.9	4.0	1.5
	7 vs 8	TX/Fed	1.9	1.2	1.4
EVAP SYS[3]	1 vs 3	DIS/As-Rec[6]	5.6	3.0	1.1
	2 vs 4	DIS/As-Rec	1.5	0.5	1.1
	6 vs 7	DIS/As-Rec	30.7	13.6	7.3

1. Fuel type comparison.
2. Temperature conditions comparison.
3. Evaporative emissions control system comparison.
4. Fed/TX refers to comparison of Federal test fuel to Texas-specific test fuel
5. TX/Fed refers to comparison of Texas-specific temperature conditions to Federal test procedure test conditions.
6. DIS/As-Rec refers to comparison of disabled evaporative emissions control system to "as-received" evaporative emissions control system.

Fuel RVP Impacts

An evaluation of fuel effects on evaporative emissions was performed using Experiments 5 and 6. As anticipated, emissions increased with RVP value. The Federal test fuel had a measured RVP value of 8.9 psia while the Houston area nonattainment ozone season fuel had an RVP value of 7.0 psia. As can be seen, increasing fuel RVP from 7.0 to 8.9 psia had significant impacts on emissions with the emissions ratio between the two experiments ranging from 5.1 to 27.4 for all three emissions categories. These results support the commonly-held opinion that decreased gasoline volatility, as measured through RVP, will result in decreased evaporative total VOC emissions.

Temperature Impacts

Three different experiment combinations could be used to evaluate temperature impacts. For all combinations, evaporative emissions generated during Texas summertime conditions exceeded emissions generated during Federal test conditions. Specifically, emissions for Texas-specific conditions ranged from 1.2 to 23.5 times higher than Federal test condition emissions. While the Texas conditions selected for evaluation may be considered to be extreme, i.e., hot soak and running loss temperatures of 105 °F and a diurnal temperature range of 72 to 105 °F, the intent of the assessment of emissions at these temperatures was to determine how large an impact temperature deviation from federal test conditions might have. Although these temperatures may not be encountered on a daily basis in Texas during the summer ozone season, it is a common occurrence to have daily maximum temperatures in excess of 95 °F. Therefore, it is

important to have an understanding of the level of significance that environmental conditions in excess of the federal test condition may have on evaporative emissions.

Evaporative Emissions Control System Impacts

Three experimental combinations were available to assess the relative impacts of the state of the evaporative emissions system. With the exception of the Experiment 2 vs 4-Hot Soak comparison, all other comparisons revealed that disabled evaporative emissions control system resulted in increased emissions relative to "as-received" emissions. Disablement of Vehicle B's system, which due to relative age of the two vehicles used is expected to be more effective in controlling emissions, resulted in significantly higher relative emissions than Vehicle A. Vehicle A disabled-to-as-received evaporative emissions ratio ranged from 1.1 to 5.6 (disregarding Experiment 2 vs 4, hot soak) while the same ratio for Vehicle B ranged from 7.3 to 30.7.

5.2.2. MOBILE6 Evaporative Emissions Assessment

EPA's MOBILE emissions model was used to generate motor vehicle emissions and have the capability of estimating evaporative emissions. As part of this research, the MOBILE6 model was used to generate emissions for each of the eight experimental conditions so that model-predicted emissions could be compared to the measured emission. To facilitate this comparison a spreadsheet model was developed utilizing information contained within MOBILE6 documentation.

SHED-measured and MOBILE6-predicted emissions for each experiment and evaporative emissions category are provided in Table 5-11.

Table 5-11. Measured vs. MOBILE-Predicted Emissions Summary.

Experiment	Source	Running Loss (g/mi)	Hot Soak (g/test)	Diurnal (g/test)
1	Measured	2.66	2.26	26.47
	Predicted	2.6	0.45	5.90
2	Measured	18.37	53.20	37.68
	Predicted	8.0	0.50	16.9
3	Measured	14.92	6.71	28.04
	Predicted	4.7	9.7	17.85
4	Measured	28.14	26.93	41.58
	Predicted	9.4	16.1	49.79
5	Measured	7.13	3.69	13.32
	Predicted	2.6	0.45	5.90
6	Measured	0.26	0.29	2.59
	Predicted	1.1	0.40	3.17
7	Measured	7.97	3.95	18.80
	Predicted	1.9	3.30	9.26
8	Measured	14.78	4.64	26.97
	Predicted	3.6	18.3	18.3

Over all eight experiments, measured emissions were greater than model-predicted in 20 of 24 possible comparisons. The average measured:predicted emission ratio over all 24 comparisons was 6.7:1. Of the three different types of evaporative emissions, the diurnal measured:predicted ratio of 2.0:1 was closest to 1:1, indicating that, on average, MOBILE6 only underpredicted emissions by a factor of 2. For hot soak and running loss emissions, the measured:predicted ratios were 15:1 and 2.6:1,

respectively. A hypothesis test on equality of means for each evaporative emission category was completed and indicated that the measured and predicted emissions were not significantly greater than predicted with a level of confidence of 95% ($\alpha = 0.05$). While it is understood that definitive conclusions associated with this work may not be possible given the limited number of experiments completed, the author believes that the results can provide insights as to the relative importance of the various parameters evaluated and information related to the potential magnitude of emissions.

Running Losses

Measured running loss emissions exceeded model-predicted emissions in seven of eight experiments. Measured and model-predicted emissions followed same trends in terms of emissions increasing with increased temperature and RVP. However, model-predicted emissions did not appear to predict the same magnitude of emissions increase as those measured, e.g., Experiment 2 vs. 1 which compared impacts of elevated temperature on emissions.

Hot Soak

Model-predicted hot soak emissions were sensitive to both temperature and fuel volatility and vehicle age. Differences due to temperature are evident by comparing Experiments 1 and 2, which indicate that as temperature increases, the model also predicts an increase in hot soak emissions, i.e., from 0.45 to 0.50 g/test or an

approximate 10% increase. Actual measured hot soak emissions also increased but the increase was a factor of 23.5 x increasing from 2.3 to 53 g/test.

Fuel volatility impacts on hot soak emissions were also evaluated. In the pair of experiments (5 and 6), decreasing fuel RVP from 8.9 to 7 psi resulted in model-predicted hot soak emissions from 0.45 to 0.40 g/test. Measured emission reductions over this change in RVP were 3.69 to 0.29 g/test, indicating a much higher sensitivity to reductions in RVP than predicted.

Diurnal losses

Temperature impacts on diurnal losses can be evaluated by comparing Experiments 1 and 2. While both temperature profiles had initial temperatures of 72 °F, the federal test procedure had maximum temperature of 96 °F and the Texas profile had a maximum temperature of 105 °F. Model-predicted diurnal emissions associated with an increase in maximum daily temperature from 96 to 105 °F increased from 5.1 to 17 g/test. Although the relative increase in model-predicted emissions (3.3 x) was larger than the relative increase in measured emissions (1.4 x), the absolute emissions measured were much larger than predicted for either temperature profile, i.e., measured greater than 2 x predicted.

Evaporative emissions control system status

Both vehicles were tested with their evaporative emissions control system functioning and disabled in order to determine relative and absolute impacts on emissions. Disabling of the evaporative emissions system was accomplished by either

disconnecting the fuel-to-canister vent line (Vehicle A) or by blocking the canister purge line (Vehicle B). The end result in either of these methods is to render the evaporative emissions control system inoperative, thus resulting in uncontrolled evaporative emissions from both vehicles.

Motor vehicle emissions testing includes a test procedure to determine the status of the evaporative emissions system. This test includes two components, a pressure test and a purge test. For the pressure test, the vehicle fuel tank and vent line are pressurized to 14 inches water column and then monitored for two minutes for pressure loss. If the system pressure does not drop below eight inches of water, the system passes. For the purge test, the vehicle is operated on a dynamometer and the canister purge rate is measured. To pass the purge test, at least one liter of air must be pulled through the canister. Vehicle A was disabled in such a manner as to be classified as a Fail Pressure Test, Vehicle B would be classified as a Fail Purge Test. Both failure modes are included in MOBILE6 emissions estimates.

Diurnal losses are predicted to increase with a failed pressure or purge test. However in two of the three comparisons, the model underpredicts diurnal losses (Experiments 3 and 7). As seen in Experiments 1 vs. 3 and 2 vs. 4, and 6 vs. 7, MOBILE6 does predict hot soak emissions to increase with a disabled evaporative emissions control system. The average measured:predicted hot soak emissions for these three experiments (3, 4 and 7) was 1.2:1.

5.2.3. A Comparison of Typical Daily Evaporative Emissions

As a means of comparison, emissions associated with a "typical" daily use pattern were generated to allow for a more tangible assessment. For this assessment, it was assumed that a total of 33 miles would be driven daily (based on an annual average rate of 12,000 miles). During this representative day, 4 complete hot soak events and the equivalent of one diurnal event were also assumed to take place. Measured vs. model-predicted emissions for this hypothetical day are provided in Table 5-12.

For 7 of 8 experiments, the measured emissions exceeded predictions. For the normal functioning vehicle experiments, i.e., Experiments 1, 2, 5 and 6, the measured emissions exceeded predicted emissions ranging from 0.3 x (Experiment 6) to as high as 3.0 x (Experiment 2). For the disabled experiments, i.e., Experiments 3, 4, 7, and 8, the measured emissions were higher than model-predicted emissions and ranged from 2.5 x (Experiment 8) to 3.5 x (Experiment 7).

Table 5-12. A Comparison of "Typical" Daily Measured and Predicted Emissions.

Experiment	Measured emissions (g/d)	Predicted emissions (g/d)
1	123	92.6
2	857	283
3	547	212
4	1078	424
5	263	93.5
6	12.3	41.1
7	298	85.2
8	533	210

Results of this analysis highlight the problem that MOBILE6 may tend to significantly underestimate evaporative emissions. A comparison of the relative

significance of emission types based on untampered typical daily average values is provided in Table 5-13.

Table 5-13. Refueling and Evaporative Emissions Relative Significance Comparison.

Parameter	Emissions (g/day)
Total evaporative emissions	325
Refueling[1]	12 (3.7%)
Running Loss	234 (72%)
Hot Soak	59 (18.2)
Diurnal	20 (6.1)

1. Refueling emissions calculated assuming 33 miles per day, 20 miles per gallon and 7.0 g VOC/gallon dispensed.

As can be seen from Table 5-13, running loss evaporative emissions are the most significant evaporative emissions source for the experiments conducted as part of this research.

5.2.4. Speciated Emissions

An evaporative emissions speciation model (Texas EVAPorative emissions model, TEVAP) was developed which allows for the calculation of speciated emissions for running loss, hot soak, diurnal and resting loss emissions. Information required to complete model execution includes:

- ambient temperatures
- liquid gasoline Reid vapor pressure (RVP)
- liquid gasoline speciated composition

The model is based primarily on an assumption of liquid-vapor equilibrium, but adjusted for differences in liquid-to-vapor mass transfer rates using the ratio of compound-specific molecular gas-phase diffusivities (to the first power). A detailed description of the model is provided in Appendix B. Speciation profiles were developed for both test gasolines by ATL and are provided in Appendix C.

A comparison of the predictive capabilities of the TEVAP Speciation Model was performed using data from Experiment 1. For each experiment, individual compound concentrations measured by ATL were converted and sorted according to percent by mass concentrations. The top 20 compounds identified and quantified were used in the model comparison. For each experiment and emissions category, the model was executed using conditions identical to those reported by ATL, e.g., Experiment 1, running loss emissions calculated using a temperature of 95 °F, Experiment 1 diurnal emissions calculated using a temperature range of 72 to 96 °F.

Model-predicted speciation percent by mass values were compared to the measured “top 20" compounds for each experiment and emissions category. Results of these comparisons for Experiment 1 are provided in Tables 5-14 through 5-16. Similar data for Experiments 2 through 8 are provided in Appendix D.

For all three emissions categories, the “top 20” compounds accounted for 97.2 to 98.6 percent of total mass profile. For the same 20 compounds, the TEVAP model predicted a contribution ranging from 93.9 to 94.5 percent.

For all 8 experiments and three emissions categories, the measured/predicted ratio for the Top 20 compound dataset ranged between 0.93 and 1.11 and had an average value

and standard deviation values of 1.02 and 0.04, respectively. These results indicate that the model developed to predict vapor profiles was capable of tracking the actual headspace concentrations closely over the different temperatures and with different fuel compositions. Therefore it is believed that the TEVAP model could be used to generate more accurate vapor speciation profiles for these evaporative emissions categories.

Table 5-14. Measured vs TEVAP-Predicted Speciation Profiles: Expt.1 Running Loss.

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	48.35	43.58	1.11
Isobutane	24.42	18.64	1.31
Butane	10.62	14.01	0.76
n-Pentane	6.53	7.15	0.91
Toluene	2.36	3.01	0.78
2,2,4-TriMePentane	1.73	2.51	0.69
2,3-Dimethylbutane	0.95	1.22	0.78
2-Methylpentane	0.63	0.85	0.74
2,3,4-Trimethylpentane	0.57	0.75	0.75
Propane	0.47	0.00	
t-2-butene	0.42	0.39	1.07
3-Methylpentane	0.28	0.42	0.69
n-Hexane	0.25	0.43	0.57
2,4-Dimethylpentane	0.19	0.37	0.52
2,4-Dimethylhexane	0.18	0.14	1.27
2,2-dimethylbutane	0.17	0.21	0.82
Cyclopentane	0.12	0.30	0.38
2,5-Dimethylhexane	0.12	0.15	0.75
Methylcyclopentane	0.10	0.25	0.40
2,3-Dimethylhexane	0.09	0.12	0.80
Total	98.55	94.51	
Average			1.04

Table 5-15. Measured vs TEVAP-Predicted Speciation Profiles: Expt.1 Hot Soak.

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Butane	65.06	14.01	4.64
Isopentane	12.87	43.58	0.30
Toluene	7.55	3.01	2.51
Isobutane	3.81	18.64	0.20
n-Pentane	2.48	7.15	0.35
2,2,4-TriMePentane	1.64	2.51	0.66
2,3,4-Trimethylpentane	0.71	0.75	0.95
2,3-Dimethylbutane	0.63	1.22	0.52
2-Methylpentane	0.41	0.85	0.49
1,2,4-Trimethylbenzene	0.38	0.05	7.19
1-Methyl-3-Ethylbenzene	0.25	0.04	5.81
n-Hexane	0.23	0.43	0.53
t-2-butene	0.22	0.39	0.56
2,4-Dimethylhexane	0.21	0.14	1.54
3-Methylpentane	0.21	0.42	0.50
2,4-Dimethylpentane	0.18	0.37	0.48
Propane	0.15	0.00	0.00
Benzene	0.15	0.10	1.44
2,5-Dimethylhexane	0.14	0.15	0.89
2,3-Dimethylhexane	0.14	0.12	1.18
Total	97.43	93.94	
Average			1.04

Table 5-16. Measured vs TEVAP-Predicted Speciation Profiles: Expt.1 Diurnal.

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	36.96	43.10	0.86
Isobutane	26.63	19.37	1.38
Butane	11.45	14.35	0.80
n-Pentane	6.46	7.00	0.92
Toluene	5.82	2.68	2.17
2,2,4-TriMePentane	3.17	2.27	1.40
2,3-Dimethylbutane	1.32	1.16	1.14
2,3,4-Trimethylpentane	1.08	0.67	1.61
2-Methylpentane	0.86	0.81	1.07
Propane	0.52	0.00	
n-Hexane	0.47	0.41	1.15
3-Methylpentane	0.43	0.39	1.10
t-2-butene	0.43	0.40	1.07
2,4-Dimethylpentane	0.40	0.34	1.16
Methylcyclopentane	0.27	0.23	1.13
2,5-Dimethylhexane	0.21	0.14	1.53
2,3-Dimethylpentane	0.19	0.15	1.30
2,2-dimethylbutane	0.19	0.20	0.91
Cyclopentane	0.17	0.29	0.59
Cyclohexane	0.17	0.15	1.13
Total	97.20	94.12	
Average			1.03

6. POTENTIAL OZONE FORMATION IMPLICATIONS

6.1. Ozone Formation Potential

The potential impacts that refueling and evaporative VOC emissions have on ozone formation were evaluated through the use of maximum incremental reactivity (MIR) values that quantify the maximum potential quantity of ozone formed by each individual VOC, expressed as g O_3 / g VOC (Carter, 1998). These values were developed to predict the ozone formation potential associated with individual VOCs under conditions in which VOCs are the rate-limiting substrate. As such, MIR values are useful for conservatively predicting the sensitivity of ozone formation to changes in VOC emissions and speciation profiles and subsequent changes in ambient VOC concentrations.

6.1.1. Refueling Emissions Impacts

Refueling experiments 7 – 12 were used to develop a measured average summer season refueling emissions rate of 7.7 g VOC / gal (Table 6.1). Predicted refueling emissions were calculated using conditions measured during Experiments 7 through 12. The predicted average summer season refueling emissions rate of 4.8 g VOC / gal.

Table 6-1. Model input data and predicted emissions estimates results.

Expt. No.	Temperature (°F) T_d[1]	T_t[2]	T_a[3]	RVP[4]	Emissions (g/gal) Measured	Predicted Mobile5a[5]
7	91	94	95	9.6	7.2	5.2
8	91	93	95	9.3	5.8	5.1
9	86	92	95	8.4	10.4	4.7
10	86	87	85	9.5	8.0	4.4
11	91	94	95	10.0	9.2	5.4
12	86	85	86	8.2	5.7	3.8
Average					**7.7 $\pm$ 1.9**	**4.8 $\pm$ 0.6**

1. Td = liquid gasoline dispensed temperature.
2. Tt = gasoline tank vapor temperature.
3. Ta = ambient temperature.
4. RVP = Reid vapor pressure (psia).
5. Mobile5a emissions estimated using "temperature-adjusted" AP-42 equation.

The average summer season refueling speciation profile, compound-specific MIR values, and the resultant ozone formation potential for each compound and the total mixture is included in Table 6.2. The speciated concentrations comprised 93.3% of the total mass quantified, or 1.30 of the 1.39 g VOC / L vapor. Multiplying each individual compound concentration by its MIR value and then adding all MIR values resulted in a total of 4.66 g O_3 / L vapor. Assuming an equivalent ratio of speciated:total MIR for the unidentified fraction, e.g., remaining 6.67%, as that for speciated VOCs results in a total of 5.0 g O_3 / L vapor. Dividing total MIR by total VOC concentrations results in 3.6 g O_3 / g VOC emitted. Finally, multiplying the average refueling emissions rate of 7.7 g VOC / gal by 3.6 g O_3 / g VOC results in a potential of 27.7 g O_3 formed / gallon of gasoline dispensed.

Table 6-2. Ozone Formation Potential Using Measured VOC Refueling Emissions and Measured Speciation Profile.

Target Compound	Ave. Refueling Conc (ug/L)	MIR[1] g O3/g VOC	MIR g O3 / L
Propane	4.71E+02	0.64	3.02E-04
2-Methylpropane	2.09E+04	1.56	3.26E-02
Butane	1.30E+05	1.44	1.87E-01
2-Methylbutane	4.15E+05	1.93	8.00E-01
1-Pentene	2.27E+04	8.16	1.86E-01
2-Methyl-1-Butene	3.93E+04	7.14	2.81E-01
Pentane	1.81E+05	1.74	3.15E-01
Trans-2-Pentene	4.45E+04	10.64	4.73E-01
Cis-2-Pentene	2.45E+04	10.62	2.60E-01
2-Methyl-2-Butene	6.54E+04	17.11	1.12E+00
2,2-Dimethylbutane	1.19E+04	1.52	1.81E-02
Cyclopentane	4.68E+03	2.61	1.22E-02
MTBE	5.70E+04	1.34	7.64E-02
2-Methylpentane	8.06E+04	2.07	1.67E-01
3-Methylpentane	4.09E+04	2.33	9.52E-02
Hexane	2.38E+04	1.69	4.03E-02
Methylcyclopentane	1.71E+04	2.4	4.11E-02
2,4-Dimethylpentane	5.16E+03	1.85	9.55E-03
Benzene	1.53E+04	1	1.53E-02
2,2,4-Trimethylpentane	1.43E+04	1.69	2.42E-02
Heptane	3.15E+03	1.43	4.51E-03
Toluene	1.33E+04	4.19	5.58E-02
Octane	3.16E+02	1.24	3.92E-04
Ethylbenzene	1.20E+03	2.97	3.57E-03
m/p-Xylene[2]	3.96E+03	7.75	3.07E-02
Styrene	2.76E+02	2.52	6.95E-04
o-Xylene	1.55E+03	7.83	1.22E-02
Nonane	1.11E+02	1.07	1.18E-04
Isopropylbenzene	1.69E+02	2.48	4.20E-04
1,3,5-Trimethylbenzene	4.39E+02	11.1	4.87E-03
Decane	4.38E+02	0.93	4.08E-04
o-Cresol[3]	0.00E+00	2.42	0.00E+00
m/p-Cresol[3]	0.00E+00	2.42	0.00E+00
Undecane	1.02E+01	0.82	8.40E-06
Napthalene	6.24E+01	3.05	1.90E-04
Dodecane	2.35E+01	0.72	1.69E-05
Tridecane	2.18E+01	0.66	1.44E-05

Table 6-2. Ozone Formation Potential Using Measured VOC Refueling Emissions and Measured Speciation Profile.

Target Compound	Ave. Refueling Conc (ug/L)	MIR[1] g O3/g VOC	MIR g O3 / L
Biphenyl[4]	9.91E+00	1	9.91E-06
Tetradecane	6.90E+00	0.6	4.14E-06
3-methyl-1-butene	8.68E+03	8.06	7.00E-02
4-methylpentane	7.98E+03	6.65	5.31E-02
1-hexene	2.39E+04	6.3	1.51E-01
trans-2-hexene	5.45E+03	8.46	4.61E-02
cis-2-hexene	5.65E+03	8.46	4.78E-02
3,3-dimethylpentane	8.49E+02	1.56	1.32E-03
2-methylhexane	7.68E+03	1.78	1.37E-02
1-heptene	1.33E+03	5.07	6.73E-03
2-methylheptane	1.04E+03	1.54	1.61E-03
3,3/3,5-dimethylheptane[5]	3.33E+01	2.16	7.19E-05
3-methyloctane[6]	2.27E+01	1.39	3.16E-05
Total speciated	1.30E+06		4.66E+00
Total VOC	1.39E+06		
UNID	9.28E+04		
Percentage of VOC speciated	93.3		
Total g O_3/ L VOC vapor			5.0
Total g O_3 / g VOC			3.6
Refueling Emissions g VOC / gal	7.7		
Refueling Emissions g O_3 / gal			27.7

1. MIR = Maximum ozone reactivity. Values obtained from Carter (1998).
2. Arithmetic average of m-xylene (11.06) and p-xylene (4.44) MIR values.
3. Assigned alkl phenols MIR value.
4. Assigned benzene MIR value.
5. Assigned 3,5-dimethylheptane MIR value.
6. Assigned arithmetic average of 2-methylheptane (1.22) and 4-methylheptane (1.55) MIR values.

A similar procedure was used to quantify the maximum ozone formation potential associated with MOBILE-based refueling emissions estimates and use of the SOSVAP speciation profile (Table 6.3). The maximum ozone formation potential associated with the use of MOBILE5a and a speciation profile not specific for the area of concern was calculated to be 16.3 g O_3 / gallon of fuel dispensed. Thus, the predicted refueling

emissions result in an underestimation of ozone formation by as much as 40%. This underscores the need to develop accurate refueling emissions inventories based on local speciation profiles.

Table 6-3. Ozone Formation Potential Using MOBILE5a-Predicted VOC Refueling Emissions and Default Speciation Profile.

Compound	MIR g O3/g VOC	SOSVAP Mass percentage	MIR g O3 /g VOC
C2CMPD[1]	9.97	0.21	2.1E-02
C3CMPD[2]	12.44	1	1.2E-01
Ethane	0.35	0.2	7.0E-04
Ethene	9.97	0.01	1.0E-03
Acetylene	1.23	0	0.0E+00
Propane	0.64	0.89	5.7E-03
Propene	12.44	0.11	1.4E-02
Isobutane	1.56	4.83	7.5E-02
1-butene/1-butylene[3]	10.8	0.9	9.7E-02
Butane	1.44	20.86	3.0E-01
t-2-butene	14.52	1.49	2.2E-01
c-2-butene	13.8	1.37	1.9E-01
3-methyl-1-butene	8.06	0.52	4.2E-02
isopentane	1.93	28.04	5.4E-01
Pentene	8.16	1.21	9.9E-02
Pentane	1.74	7.51	1.3E-01
isoprene	11.47	0.07	8.0E-03
t-2-pentene	10.64	2.35	2.5E-01
c-2-pentene	10.62	1.28	1.4E-01
2-methyl-2-butene	17.11	3.24	5.5E-01
2,2-dimethylbutane	1.52	0.72	1.1E-02
cyclopentene	2.74	0.39	1.1E-02
4-methyl-1-pentene	6.65	0.25	1.7E-02
cyclopentane	2.61	0.45	1.2E-02
3-methylpentane	2.33	2.1	4.9E-02
2-methylpentane	2.07	3.81	7.9E-02
2,3,dimethylbutane	1.31	1.62	2.1E-02
2-methyl-1-pentene	5.43	0.29	1.6E-02
Hexane	1.69	1.3	2.2E-02
t-2-hexene	8.46	0.32	2.7E-02

Table 6-3. Ozone Formation Potential Using MOBILE5a-Predicted VOC Refueling Emissions and Default Speciation Profile.

c-2-hexene	8.46	0.18	1.5E-02
methylcyclopentane	2.4	0.9	2.2E-02
2,4-dimethylpentane	1.85	0.66	1.2E-02
benzene	1	0.97	9.7E-03
cyclohexane	1.96	0.13	2.5E-03
2-methylhexane	1.78	0.57	1.0E-02
2,3,dimethylpentane	1.78	0.65	1.2E-02
3-methylhexane	2.22	0.55	1.2E-02
2,2,4-trimethylpentane	1.69	1.56	2.6E-02
Heptane	1.43	0.28	4.0E-03
methylcyclohexane	2.11	0.13	2.7E-03
2,3,4-trimethylpentane	1.52	0.42	6.4E-03
Toluene	4.19	1.93	8.1E-02
2-methylheptane	1.54	0.9	1.4E-02
3-methylheptane	1.78	0.03	5.3E-04
Octane	1.24	0.6	7.4E-03
ethylbenzene	2.97	0.2	5.9E-03
m,p-xylenes[4]	7.75	0.62	4.8E-02
Styrene	2.52	0.02	5.0E-04
o-xylene	7.83	0.22	1.7E-02
Nonane	1.07	0.02	2.1E-04
isopropylbenzene	2.48	0.03	7.4E-04
n-propylbenzene	2.35	0.04	9.4E-04
1,3,5-trimethylbenzene	11.1	0.06	6.7E-03
1,2,4-trimethylbenzene	7.49	0.18	1.3E-02
UNID		3.37	
Total		102.56	3.4E+00
Percentage of VOC speciated		99.19	
Total g O3/g VOC			3.4
Refueling Emissions g VOC / gal[5]			4.8
Refueling Emissions g O_3 / gal			16.3

1. Assigned Ethene MIR value.
2. Assigned Propene MIR value.
3. Assigned butene MIR value.
4. Assigned arithmetic average of m- and p-xylene MIR values
5. MOBILE-5a average refueling emissions value obtained from Table 6.1

6.1.2. Evaporative Emissions Impacts

Running loss, hot soak, and diurnal evaporative emissions impacts on ozone formation potential were also evaluated. This evaluation included the comparison of ozone formation potential associated with measured emissions and predicted emissions. SHED evaporative experiments 1 through 8 served as the basis of this evaluation. Due to the large differences in emissions between the vehicles with operating evaporative emissions systems (Experiments 1,2, 5 and 6) and disabled evaporative emissions systems (Experiments 3, 4, 7 and 8), two evaluations were completed; one for the non-tampered (NORMAL) system experiments, and one for tampered (HIGH EMITTER) system experiments.

NORMAL System Evaporative Emissions Impacts

An average NORMAL running loss, hot soak and diurnal emission rate was calculated from Experiment 1, 2, 5, and 6 results (Table 6.4).

Table 6-4. Measured NORMAL System Running Loss, Hot Soak and Diurnal Total VOC Emissions

Experiment	Running Loss (g/mi)[1]	Hot Soak (g/test)[2]	Diurnal (g/test)[3]
1	2.66	2.26	26.47
2	18.37	53.20	37.68
5	7.13	3.69	13.32
6	0.26	0.29	2.59
Average	**7.11 ± 8.03**	**14.9 ± 25.6**	**20.0 ± 15.3**

1. Running loss emissions were calculated as the total mass measured in SHED divided by total dynamometer miles traveled.
2. Hot soak emissions were quantified at the end of the 1-hour hot soak test.
3. Diurnal emissions were quantified at the end of the 24-hour diurnal test.

Average speciation profiles for each emissions type were also determined for the NORMAL systems experiments. Ozone formation potential for each profile and for each emissions rate were calculated as generally described in Section 6.2. Average running loss, hot soak and diurnal speciation profiles and the ozone formation potential for each profile are provided in Tables 6-5 through 6-7.

Table 6-5. Average Measured NORMAL Running Loss Speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.485	1.93	0.936
Isobutane	0.151	1.56	0.236
Butane	0.075	1.44	0.107
n-Pentane	0.085	1.74	0.147
Toluene	0.022	4.19	0.091
2,2,4-TriMePentane	0.023	1.69	0.038
2,3-Dimethylbutane	0.015	1.31	0.020
2-Methylpentane	0.015	2.07	0.032
2,3,4-Trimethylpentane	0.007	1.52	0.010
Propane	0.003	0.64	0.002
t-2-butene	0.007	14.52	0.097
3-Methylpentane	0.008	2.33	0.018
n-Hexane	0.007	1.69	0.012
2,4-Dimethylpentane	0.003	1.85	0.006
2,4-Dimethylhexane	0.001	2.31	0.002
2,2-dimethylbutane	0.003	1.52	0.005
Cyclopentane	0.000	2.61	0.001
2,5-Dimethylhexane	0.001	2.21	0.001
Methylcyclopentane	0.004	2.4	0.010
2,3-Dimethylhexane	0.001	1.78	0.001
m-Xylene	0.004	11.06	0.045
Cyclohexane	0.000	1.96	0.001
2-Methylhexane	0.001	1.78	0.001
2,3-Dimethylpentane	0.001	1.78	0.001
3-Methylhexane	0.001	2.22	0.002
Benzene	0.002	1	0.002
cis-2-Pentene	0.001	10.62	0.016
1-Butene	0.001	10.8	0.015
cis-2-Butene	0.003	13.8	0.036
trans-2-Pentene	0.004	10.64	0.038
MTBE	0.013	1.34	0.018
1,2,4-Trimethylbenzene	0.000	2.35	0.000
1-Methyl-3-Ethylbenzene	0.000	6.9	0.000
o-Xylene	0.000	7.83	0.000
Ethylbenzene	0.000	2.97	0.000
2-methyl-2-butene	0.000	5.06	0.000
trans-2-Hexene	0.000	8.46	0.000
1-methylcyclopentene	0.000	2.74	0.000
1-Hexene	0.000	6.3	0.000
Speciated Total	0.945		
Adjusted O3 total (g O3/g total VOC)			**2.06**

1. OFP - Ozone Formation Potential

Table 6-6. Average Measured NORMAL Hot Soak Speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.291	1.93	0.563
Isobutane	0.079	1.56	0.124
Butane	0.198	1.44	0.285
n-Pentane	0.062	1.74	0.109
Toluene	0.073	4.19	0.307
2,2,4-TriMePentane	0.026	1.69	0.043
2,3-Dimethylbutane	0.015	1.31	0.019
2-Methylpentane	0.016	2.07	0.032
2,3,4-Trimethylpentane	0.007	1.52	0.011
Propane	0.001	0.64	0.001
t-2-butene	0.001	14.52	0.019
3-Methylpentane	0.008	2.33	0.019
n-Hexane	0.009	1.69	0.015
2,4-Dimethylpentane	0.004	1.85	0.007
2,4-Dimethylhexane	0.002	2.31	0.004
2,2-dimethylbutane	0.001	1.52	0.001
Cyclopentane	0.000	2.61	0.000
2,5-Dimethylhexane	0.001	2.21	0.003
Methylcyclopentane	0.006	2.4	0.014
2,3-Dimethylhexane	0.000	1.78	0.001
m-Xylene	0.014	11.06	0.151
Cyclohexane	0.001	1.96	0.002
2-Methylhexane	0.003	1.78	0.006
2,3-Dimethylpentane	0.001	1.78	0.002
3-Methylhexane	0.003	2.22	0.007
Benzene	0.011	1	0.011
cis-2-Pentene	0.003	10.62	0.028
1-Butene	0.000	10.8	0.000
cis-2-Butene	0.000	13.8	0.000
trans-2-Pentene	0.006	10.64	0.063
MTBE	0.019	1.34	0.026
1,2,4-Trimethylbenzene	0.008	2.35	0.018
1-Methyl-3-Ethylbenzene	0.005	6.9	0.032
o-Xylene	0.005	7.83	0.040
Ethylbenzene	0.003	2.97	0.010
2-methyl-2-butene	0.003	5.06	0.014
trans-2-Hexene	0.002	8.46	0.019
1-methylcyclopentene	0.000	2.74	0.000
1-Hexene	0.000	6.3	0.000
Speciated Total	0.886		
Adjusted O3 total (g O3/g total VOC)			**2.26**

1. OFP - Ozone Formation Potential

Table 6-7. Average Measured NORMAL Diurnal Speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.339	1.93	0.654
Isobutane	0.200	1.56	0.312
Butane	0.084	1.44	0.121
n-Pentane	0.069	1.74	0.120
Toluene	0.057	4.19	0.238
2,2,4-TriMePentane	0.030	1.69	0.050
2,3-Dimethylbutane	0.011	1.31	0.015
2-Methylpentane	0.017	2.07	0.036
2,3,4-Trimethylpentane	0.006	1.52	0.010
Propane	0.009	0.64	0.006
t-2-butene	0.006	14.52	0.081
3-Methylpentane	0.009	2.33	0.020
n-Hexane	0.008	1.69	0.014
2,4-Dimethylpentane	0.003	1.85	0.005
2,4-Dimethylhexane	0.000	2.31	0.000
2,2-dimethylbutane	0.001	1.52	0.002
Cyclopentane	0.001	2.61	0.002
2,5-Dimethylhexane	0.001	2.21	0.002
Methylcyclopentane	0.006	2.4	0.015
2,3-Dimethylhexane	0.000	1.78	0.000
m-Xylene	0.005	11.06	0.052
Cyclohexane	0.001	1.96	0.002
2-Methylhexane	0.003	1.78	0.005
2,3-Dimethylpentane	0.001	1.78	0.003
3-Methylhexane	0.002	2.22	0.005
Benzene	0.008	1	0.008
cis-2-Pentene	0.004	10.62	0.044
1-Butene	0.000	10.8	0.000
cis-2-Butene	0.000	13.8	0.000
trans-2-Pentene	0.000	10.64	0.000
MTBE	0.027	1.34	0.036
1,2,4-Trimethylbenzene	0.000	2.35	0.000
1-Methyl-3-Ethylbenzene	0.000	6.9	0.000
o-Xylene	0.000	7.83	0.000
Ethylbenzene	0.000	2.97	0.000
2-methyl-2-butene	0.000	5.06	0.000
trans-2-Hexene	0.003	8.46	0.022
1-methylcyclopentene	0.002	2.74	0.006
1-Hexene	0.002	6.3	0.015
Speciated Total	0.914		
Adjusted O3 total (g O3/g total VOC)			**2.08**

1. OFP - Ozone Formation Potential

Table 6-8. Predicted NORMAL System Running Loss, Hot Soak and Diurnal Total VOC Emissions

Experiment	Running Loss (g/mi)[1]	Hot Soak (g/test)[2]	Diurnal (g/test)[3]
1	2.6	0.45	5.90
2	8.0	0.50	16.9
5	2.6	0.45	5.90
6	1.1	0.40	3.17
Average	**3.58 $\pm$ 3.99**	**0.45 $\pm$ 0.04**	**7.97 $\pm$ 6.09**

1. Running loss emissions were calculated as the total mass measured in SHED divided by total dynamometer miles traveled.
2. Hot soak emissions were quantified at the end of the 1-hour hot soak test.
3. Diurnal emissions were quantified at the end of the 24-hour diurnal test.

The ozone formation potential resulting from either use of measured or predicted data are provided in Table 6-9. The SOSVAP speciation profile (Table 6.3) was used in the calculation of predicted ozone formation potential. Ozone formation potential associated with measured data exceeded that calculated using model-predicted emissions and a default speciation profile, ranging from 1.2 times as high for running emissions to greater than 22 times as high for hot soak emissions. The primary reason for these differences can be attributed to the differences in the measured vs. predicted emissions rate.

A hypothesis test on equality of means indicated that the measured and predicted emissions were not significantly different (level of confidence of 95%, $\alpha = 1$). While the limited number of experiments completed may not be sufficient to result in statistical-based difference significance, comparing the overall trends in the experiments does indicate that the measured vs predicted ozone formation potentials may be different.

Table 6-9. NORMAL System: Measured vs. Predicted Ozone Formation

	Measured	Predicted
Running Loss		
Average Emissions (g VOC/mile)	7.11 ± 8.03	3.58 ± 3.99
OFP (g O_3 / g total VOC)	2.06	3.4
OFP (g O_3/ mi)	14.6	12.2
Hot Soak		
Average Emissions (g VOC/test)	14.9 ± 25.6	0.45 ± 0.04
OFP (g O_3 / g total VOC)	2.26	3.4
OFP (g O_3/ test)	33.7	1.53
Diurnal		
Average Emissions (g VOC/test)	20.0 ± 15.3	7.97 ± 6.09
OFP (g O_3 / g total VOC)	2.08	3.4
OFP (g O_3/ test)	41.6	27.1

HIGH EMITTER System Evaporative Emissions Impacts

HIGH EMITTER system emissions and subsequent potential impacts on ozone formation were evaluated in the same manner as that described in Section 6.3.1 NORMAL System Evaporative System Emissions Impacts. Tables 6-10 through 6-15 contain data used for this assessment.

A hypothesis test on equality of means indicated that the measured and predicted total VOC emissions (Table 6-10 and 6-14) were not significantly different (level of confidence of 95%, α =1).

However, results of this evaluation indicate that differences between measured and predicted impacts on ozone formation associated with HIGH EMITTERS may be large. For example, ozone formation potential associated with measured running loss evaporative emissions may be 2.5 times higher than the predicted emissions-related impacts.

Table 6-10. Measured HIGH EMITTER System Running Loss, Hot Soak and Diurnal Total VOC Emissions

Experiment	Running Loss (g/mi)[1]	Hot Soak (g/test)[2]	Diurnal (g/test)[3]
3	14.92	6.71	28.04
4	28.14	26.93	41.58
7	7.97	3.95	18.80
8	14.78	4.64	26.97
Average	**16.45 ± 8.44**	**10.56 ± 10.98**	**28.85 ± 9.44**

1. Running loss emissions were calculated as the total mass measured in SHED divided by total dynamometer miles traveled.
2. Hot soak emissions were quantified at the end of the 1-hour hot soak test.
3. Diurnal emissions were quantified at the end of the 24-hour diurnal test.

Table 6-11. Average Measured HIGH EMITTER Running Loss speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.411	1.93	0.793
Isobutane	0.085	1.56	0.132
Butane	0.052	1.44	0.075
n-Pentane	0.104	1.74	0.181
Toluene	0.023	4.19	0.095
2,2,4-TriMePentane	0.016	1.69	0.027
2,3-Dimethylbutane	0.014	1.31	0.018
2-Methylpentane	0.035	2.07	0.072
2,3,4-Trimethylpentane	0.004	1.52	0.007
Propane	0.002	0.64	0.001
t-2-butene	0.009	14.52	0.129
3-Methylpentane	0.017	2.33	0.040
n-Hexane	0.013	1.69	0.021
2,4-Dimethylpentane	0.002	1.85	0.005
2,4-Dimethylhexane	0.001	2.31	0.002
2,2-dimethylbutane	0.006	1.52	0.009
Cyclopentane	0.003	2.61	0.008
2,5-Dimethylhexane	0.001	2.21	0.002
Methylcyclopentane	0.009	2.4	0.023
2,3-Dimethylhexane	0.000	1.78	0.001
m-Xylene	0.000	11.06	0.000
Cyclohexane	0.001	1.96	0.001
2-Methylhexane	0.002	1.78	0.004
2,3-Dimethylpentane	0.001	1.78	0.002
3-Methylhexane	0.000	2.22	0.000
Benzene	0.006	1	0.006
cis-2-Pentene	0.011	10.62	0.112
1-Butene	0.000	10.8	0.000
cis-2-Butene	0.005	13.8	0.069
trans-2-Pentene	0.023	10.64	0.249
MTBE	0.030	1.34	0.041
1,2,4-Trimethylbenzene	0.000	2.35	0.000
1-Methyl-3-Ethylbenzene	0.000	6.9	0.000
o-Xylene	0.000	7.83	0.000
Ethylbenzene	0.000	2.97	0.000
2-methyl-2-butene	0.011	5.06	0.057
trans-2-Hexene	0.004	8.46	0.037
1-methylcyclopentene	0.000	2.74	0.000
1-Hexene	0.005	6.3	0.030
1-pentene	0.002	8.16	0.017
Speciated Total	0.908		
Adjusted O3 total (g O3/g total VOC)			**2.50**

1. OFP - Ozone Formation Potential

Table 6-12. Average Measured HIGH EMITTER Hot Soak Speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.349	1.93	0.674
Isobutane	0.070	1.56	0.109
Butane	0.155	1.44	0.224
n-Pentane	0.083	1.74	0.144
Toluene	0.042	4.19	0.178
2,2,4-TriMePentane	0.023	1.69	0.039
2,3-Dimethylbutane	0.013	1.31	0.017
2-Methylpentane	0.025	2.07	0.052
2,3,4-Trimethylpentane	0.007	1.52	0.011
Propane	0.000	0.64	0.000
t-2-butene	0.005	14.52	0.079
3-Methylpentane	0.013	2.33	0.029
n-Hexane	0.010	1.69	0.017
2,4-Dimethylpentane	0.003	1.85	0.006
2,4-Dimethylhexane	0.002	2.31	0.004
2,2-dimethylbutane	0.001	1.52	0.002
Cyclopentane	0.001	2.61	0.004
2,5-Dimethylhexane	0.001	2.21	0.003
Methylcyclopentane	0.008	2.4	0.019
2,3-Dimethylhexane	0.000	1.78	0.000
m-Xylene	0.002	11.06	0.018
Cyclohexane	0.001	1.96	0.003
2-Methylhexane	0.003	1.78	0.005
2,3-Dimethylpentane	0.002	1.78	0.003
3-Methylhexane	0.000	2.22	0.000
Benzene	0.005	1	0.005
cis-2-Pentene	0.006	10.62	0.067
1-Butene	0.000	10.8	0.000
cis-2-Butene	0.003	13.8	0.041
trans-2-Pentene	0.015	10.64	0.157
MTBE	0.044	1.34	0.059
1,2,4-Trimethylbenzene	0.000	2.35	0.000
1-Methyl-3-Ethylbenzene	0.000	6.9	0.000
o-Xylene	0.000	7.83	0.000
Ethylbenzene	0.000	2.97	0.000
2-methyl-2-butene	0.007	5.06	0.037
trans-2-Hexene	0.003	8.46	0.027
1-methylcyclopentene	0.000	2.74	0.000
1-Hexene	0.003	6.3	0.021
1-pentene	0.000	8.16	0.000
Speciated Total	0.909		
Adjusted O3 total (g O3/g total VOC)			**2.26**

1. OFP - Ozone Formation Potential

Table 6-13. Average Measured HIGH EMITTER Diurnal Speciation Profile and Ozone Formation Potential

Compound	Ave. Speciation Profile g / g total VOC	MIR (g O3 / g VOC cmpd)	MIR-based OFP[1] g O3 / g total VOC
Isopentane	0.335	1.93	0.646
Isobutane	0.122	1.56	0.191
Butane	0.064	1.44	0.092
n-Pentane	0.093	1.74	0.162
Toluene	0.042	4.19	0.177
2,2,4-TriMePentane	0.026	1.69	0.044
2,3-Dimethylbutane	0.010	1.31	0.014
2-Methylpentane	0.029	2.07	0.061
2,3,4-Trimethylpentane	0.008	1.52	0.012
Propane	0.002	0.64	0.001
t-2-butene	0.009	14.52	0.135
3-Methylpentane	0.014	2.33	0.034
n-Hexane	0.011	1.69	0.018
2,4-Dimethylpentane	0.003	1.85	0.005
2,4-Dimethylhexane	0.002	2.31	0.005
2,2-dimethylbutane	0.004	1.52	0.006
Cyclopentane	0.004	2.61	0.010
2,5-Dimethylhexane	0.002	2.21	0.004
Methylcyclopentane	0.008	2.4	0.020
2,3-Dimethylhexane	0.001	1.78	0.001
m-Xylene	0.000	11.06	0.000
Cyclohexane	0.001	1.96	0.003
2-Methylhexane	0.000	1.78	0.000
2,3-Dimethylpentane	0.002	1.78	0.003
3-Methylhexane	0.000	2.22	0.000
Benzene	0.005	1	0.005
cis-2-Pentene	0.010	10.62	0.103
1-Butene	0.000	10.8	0.000
cis-2-Butene	0.005	13.8	0.069
trans-2-Pentene	0.022	10.64	0.234
MTBE	0.056	1.34	0.074
1,2,4-Trimethylbenzene	0.000	2.35	0.000
1-Methyl-3-Ethylbenzene	0.000	6.9	0.000
o-Xylene	0.000	7.83	0.000
Ethylbenzene	0.000	2.97	0.000
2-methyl-2-butene	0.010	5.06	0.052
trans-2-Hexene	0.000	8.46	0.000
1-methylcyclopentene	0.000	2.74	0.000
1-Hexene	0.004	6.3	0.026
1-pentene	0.004	8.16	0.032
Speciated Total	0.910		
Adjusted O3 total (g O3/g total VOC)			**2.46**

1. OFP - Ozone Formation Potential

Table 6-14. Predicted HIGH EMITTER System Running Loss, Hot Soak and Diurnal Total VOC Emissions

Experiment	Running Loss (g/mi)[1]	Hot Soak (g/test)[2]	Diurnal (g/test)[3]
3	4.7	9.7	17.85
4	9.4	16.1	49.79
7	1.9	3.30	9.26
8	3.6	18.3	18.3
Average	**4.9 ± 3.21**	**11.85 ± 6.77**	**23.80 ± 17.8**

1. Running loss emissions were calculated as the total mass measured in SHED divided by total dynamometer miles traveled.
2. Hot soak emissions were quantified at the end of the 1-hour hot soak test.
3. Diurnal emissions were quantified at the end of the 24-hour diurnal test.

Table 6-15. HIGH EMITTER System: Measured vs. Predicted Ozone Formation

	Measured	Predicted
Running Loss		
Average Emissions (g VOC/mile)	16.45 ± 8.44	4.9 ± 3.21
OFP (g O_3 / g total VOC)	2.50	3.4
OFP (g O_3/ mi)	41.1	16.7
Hot Soak		
Average Emissions (g VOC/test)	10.56 ± 10.98	11.85 ± 6.77
OFP (g O_3 / g total VOC)	2.26	3.4
OFP (g O_3/ test)	23.97	40.3
Diurnal		
Average Emissions (g VOC/test)	28.85 ± 9.44	23.80 ± 17.8
OFP (g O_3 / g total VOC)	2.46	3.4
OFP (g O_3/ test)	80.0	80.7

7. CONCLUSIONS AND RECOMMENDATIONS

7.1. Summary

This dissertation focused on refueling and evaporative emissions of gasoline vapors. The methodologies described herein can be employed to update emission factors as the vehicle fleet and gasoline composition changes in the future. The results described herein are representative of older vehicles in the United States. However they may be useful for current vehicle fleets in developing countries such as China and Mexico.

7.1.1. Refueling Studies

This research has resulted in a database consisting of vehicle pre-fill and refueling vapor compositions in Austin, Texas. A novel device was designed and constructed that enabled the simultaneous sampling of gasoline vapors and measurement of volumetric vapor flow rates during refueling. The device should be valuable for future studies related to uncontrolled refueling emissions. A total of 12 uncontrolled refueling events were completed and involved the determination of volumetric flow rates of gasoline vapor during refueling, as well as total and speciated VOC concentrations. Refueling emissions were determined as the product of VOC concentration (total or speciated) and volumetric flow rates of gasoline vapor. Total VOC emissions were compared with two commonly used algorithms. Speciated VOC vapor profiles were compared with two published gasoline vapor profiles and theoretical predictions based on knowledge of liquid composition and environmental conditions. An evaluation of refueling emissions impacts on ozone formation potentials using MIR was completed and results were

compared against speciated emissions and MOBILE-based total VOC emissions estimates coupled with a default speciation profile.

7.1.2. Evaporative Emissions

A model was developed to predict the speciation of VOCs associated with evaporative emissions from motor vehicles. The speciation model, TEVAP, is based on liquid-vapor equilibrium and requires liquid gasoline speciation, gasoline Reid Vapor Pressure and temperature data. Model-predicted speciation profiles were evaluated using SHED studies. A total of 8 SHED evaporative emissions tests were designed and completed to investigate the effects of Texas-specific gasoline composition, environmental conditions and evaporative emissions control system-status on evaporative emissions. Running loss, hot soak and diurnal emissions were included in each test. Total VOC emissions measured during each test were compared against MOBILE6 predicted emissions. An evaluation of evaporative emissions impacts on ozone formation potentials using MIR was completed, comparing measured speciated emissions and MOBILE6-based total VOC emissions estimates coupled with a default speciation profile.

7.2. Conclusions

7.2.1. Refueling Studies

- *It is likely that significant volume expansion occurs during mass transfer from fresh gasoline which is dispensed into a fuel tank environment containing aged gasoline vapors, a factor not generally accounted for or evaluated in previous studies*. Measured volumetric flow rates were, on average, 52% higher than those

predicted using a published algorithm. The latter was based on studies involving the discharge of fresh gasoline into fresh gasoline over a range of dispensed and residual (fuel tank) liquid temperatures.

- *On average, refueling vapor concentration is higher than pre-fill (aged) vapor concentration*.

- *Gasoline speciation profiles based on liquid composition and Raoult's law better reflect the measured vapor speciation profile than standard published profiles*. This suggests that it would be advantageous to use an area-specific liquid concentration profile and Raoult's law as a basis for estimating gasoline vapor profiles during refueling.

- *Refueling VOC emissions may be underestimated in existing emission inventories, particularly during the summer ozone season.* Measured total VOC emissions were, on average, higher than those predicted using the AP-42 refueling emission factor, the algorithm used to develop the final regulatory impact analysis for on-board refueling vapor recovery (ORVR) systems and the MOBILE5a model. During the ozone season, measured VOC emissions were, on average, 28% higher than those predicted based on AP-42 and 39% higher than those based on the ORVR model and 60% higher than MOBILE5a.

- *Refueling VOC emissions based on MOBILE may significantly underestimate ozone formation potential*. A comparison of the ozone formation potential between summer season measured refueling emissions and MOBILE5a-predicted

refueling emissions resulted in an underestimation by as much as 40% when predicted emissions are used.

7.2.2. Evaporative Emissions

- *Texas-specific environmental conditions resulted in evaporative emissions that exceed Federal test conditions*, i.e., 1.2 to 23.5 times higher.

- *Evaporative emissions increase with increased RVP for all three evaporative emissions categories.*

- *Disabled evaporative emissions control systems generally lead to much higher emissions than functioning systems.*

- *MOBILE6 may underestimate evaporative emissions of VOCs.* Measured total VOC emissions were compared to MOBILE6-predicted emissions. In 20 of 24 possible comparisons, measured exceeded predicted emissions, and over all 24 comparisons, the measured:predicted ratio was 6.7:1. Of the three different types of evaporative emissions, the measured:predicted ratio for diurnal emissions was 2:1 while the hot soak and running loss measured:predicted ratios were 15:1 and 2.6:1, respectively.

- *The MOBILE6 may not adequately capture the sensitivity of emissions to RVP and temperature parameters.* MOBILE6-predicted and measured hot soak emissions decreased with reductions in RVP and temperature. However, for the temperature and RVP comparisons tested, MOBILE6 -based hot soak emissions

were predicted to change by only approximately 10%. Measured emissions increased by more than an order of magnitude.

- *MOBILE6 may underestimate daily evaporative emissions resulting in underestimated motor vehicle evaporative emissions inventories*. Evaporative emissions associated with a "typical" day were calculated for each test scenario using measured and predicted emissions. For all scenarios, "typical" daily measured emissions exceeded predicted emissions, with measured:predicted ratios ranging from 1.5:1 to 33:1.

- *The TEVAP model developed in this study was capable of predicting vapor speciation profiles over the operating conditions tested and may be a useful tool in developing accurate vapor speciation profiles for evaporative emissions*. Measured speciation profiles for all tests and evaporative emissions categories were compared to model-predicted speciation profiles. The "top 20" compounds, as determined by concentration were used for each comparison and accounted for more than 97% of total mass in all tests. For all comparisons, the measured/predicted ratio ranged from 0.93 to 1.11 and had an average and standard deviation value of 1.02 and 0.04, respectively.

- *MOBILE6-based ozone formation potentials are likely underestimated for evaporative emissions for the normal evaporative emissions control system conditions.* For running loss, hot soak and diurnal emissions, the normal average measured:predicted MIR ratios ranged from 1.2:1 to 22:1

7.3. Recommendations

Gasoline formulations change over time, with current trends toward increased use of ethanol. Future research in this area should include the effect of ethanol on refueling and evaporative emissions as well as liquid-vapor equilibrium relationships. Specific recommendations related to refueling and evaporative emissions are presented in the following sub-sections.

7.3.1. Refueling Studies

This research has generated data indicating that current algorithms used to predict refueling emissions may underestimate emissions. Additional refueling experiments involving the dispensement of "fresh" gasoline into fuel tanks containing aged gasoline is recommended to supplement data described herein. This would allow for the potential revision of existing predictive algorithms to account for this difference in fuel compositions not previously examined in detail.

Refueling vapor data indicate that the displaced vapor composition is not simply due to the displacement of existing vapors within the tank. Liquid-to-vapor mass transfer is believed to occur as the dispensed "fresh" fuel is discharged into the tank. It is recommended that additional research be undertaken similar to the research described herein, with the exception that samples of liquid gasoline residing within the tank be collected prior to refueling and at intermediate times during refueling, to allow for the speciation and temperature of the resident fuel. This additional information would facilitate a determination of the relationships between liquid fuel composition within the tank and the displaced vapors. The result of this additional research would be an

improved refueling database which could also facilitate the development of refueling-specific vapor speciation profiles. Further these data could be used during evaluation of on-board vapor recovery systems in terms of adsorption capacity requirements to determine overall VOC removal efficiencies during extreme refueling emissions conditions, e.g., high dispensed temperature and high RVP fuels.

7.3.2. Evaporative Emissions

SHED evaporative emissions tests designed and completed for this dissertation were not robust enough to reach statistically significant conclusions, but indicate several interesting observations related to the comparisons between measured and MOBILE6-predicted emissions. It is recommended that additional SHED testing be done at elevated temperatures similar to the conditions described herein to better understand the impacts that environmental conditions, likely to be present during the summer ozone season, have on evaporative emissions. It is also recommended that further examination of MOBILE6 be undertaken in terms of sensitivity analyses and comparisons to available measured data to better understand potential model limitations.

It is recommended that consideration be given to the use of a speciation model such as TEVAP during development of area-specific evaporative emissions speciation profiles.

APPENDIX A - REFUELING EMISSIONS AND SPECIATION DATA

Table A-1. Refueling Experiment #1: Vapor Concentration and Emissions Profile

Compound	Vapor Composition (ug/L)[a]				Emissions
	Pre-Fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	0.0	814.3	1127.0	970.7	4.46E-03
2-Methylpropane	0.0	46570.4	56243.1	51406.7	2.36E-01
Butane	530.3	397967.9	492647.8	445307.9	2.04E+00
2-Methylbutane	790.7	318910.3	374835.3	346872.8	1.59E+00
1-Pentene	0.0	19888.3	23059.9	21474.1	9.86E-02
2-Methyl-1-Butene	63.5	32749.4	39077.7	35913.6	1.65E-01
Pentane	425.9	137986.6	163964.4	150975.5	6.93E-01
Trans-2-Pentene	113.9	37401.2	44251.0	40826.1	1.87E-01
Cis-2-Pentene	0.0	19066.0	22632.1	20849.0	9.57E-02
2-Methyl-2-Butene	150.4	49192.9	58932.2	54062.5	2.48E-01
2,2-Dimethylbutane	0.0	6753.2	8271.6	7512.4	3.45E-02
Cyclopentane	0.0	8507.7	10571.5	9539.6	4.38E-02
MTBE	30.7	14779.8	17550.8	16165.3	7.42E-02
2-Methylpentane	345.5	45785.1	55071.4	50428.3	2.31E-01
3-Methylpentane	208.7	22549.1	27694.4	25121.7	1.15E-01
Hexane	162.2	13974.4	18144.3	16059.3	7.37E-02
Methylcyclopentane	159.5	8850.1	11286.4	10068.2	4.62E-02
2,4-Dimethylpentane	43.5	1943.9	2627.9	2285.9	1.05E-02
Benzene	202.4	6191.9	8873.5	7532.7	3.46E-02
2,2,4-Trimethylpentane	319.0	3260.1	4363.1	3811.6	1.75E-02
Heptane	151.5	1130.6	1572.9	1351.7	6.20E-03
Toluene	1093.1	3331.9	5212.6	4272.2	1.96E-02
Octane	78.0	75.1	115.6	95.3	4.38E-04
Ethylbenzene	270.9	186.0	344.9	265.5	1.22E-03
m/p-Xylene	1263.6	745.3	1421.1	1083.2	4.97E-03
Styrene	15.6	16.0	45.4	30.7	1.41E-04
o-Xylene	467.9	220.4	439.2	329.8	1.51E-03
Nonane	0.0	0.0	0.0	0.0	0.00E+00
Isopropylbenzene	0.0	0.0	0.0	0.0	0.00E+00
1,3,5 TMB	178.8	23.6	59.7	41.7	1.91E-04
Decane	0.0	0.0	0.0	0.0	0.00E+00
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	0.0	0.0	0.0	0.0	0.00E+00
Napthalene	0.0	0.0	0.0	0.0	0.00E+00
Dodecane	0.0	0.0	0.0	0.0	0.00E+00
Tridecane	5.6	6.9	0.0	3.5	1.59E-05
Biphenyl	0.0	0.0	0.0	0.0	0.00E+00
Tetradecane	1.1	3.7	0.0	1.8	8.45E-06
THC	1.29E+04	1.33E+06	1.61E+06	1.47E+06	6.75E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor composition during refueling

[a] Concentrations in table do not reflect actual number of significant figures, but rather computer output. Concentrations can reasonably be characterized by two significant figures. This is true for all remaining tables in this appendix.

Table A-2. Refueling Experiment #2: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L) Pre-Fill (1)	Refueling (2) Sample 1	Refueling (2) Sample 2	Average Refueling	Emissions (g/gal)
Propane	0.0	644.0	966.0	805.0	3.69E-03
2-Methylpropane	3363.7	38853.9	45646.6	42250.2	1.94E-01
Butane	35221.7	363209.3	423019.5	393114.4	1.80E+00
2-Methylbutane	33453.2	276174.6	346446.7	311310.6	1.43E+00
1-Pentene	2282.5	17920.5	22180.8	20050.6	9.20E-02
2-Methyl-1-Butene	3441.8	29388.0	35861.2	32624.6	1.50E-01
Pentane	15397.1	122115.5	152506.5	137311.0	6.30E-01
Trans-2-Pentene	4502.0	34334.7	42732.1	38533.4	1.77E-01
Cis-2-Pentene	2310.6	17662.4	22071.7	19867.0	9.12E-02
2-Methyl-2-Butene	5855.1	45570.9	56932.9	51251.9	2.35E-01
2,2-Dimethylbutane	348.6	5846.4	6689.4	6267.9	2.88E-02
Cyclopentane	882.9	7657.3	9501.6	8579.4	3.94E-02
MTBE	1666.7	13628.8	17410.0	15519.4	7.12E-02
2-Methylpentane	4569.1	41289.7	51389.0	46339.4	2.13E-01
3-Methylpentane	2254.9	20702.5	25871.7	23287.1	1.07E-01
Hexane	1359.8	13558.8	16838.1	15198.5	6.98E-02
Methylcyclopentane	1042.0	8476.4	10955.7	9716.0	4.46E-02
2,4-Dimethylpentane	267.1	2062.7	2794.6	2428.6	1.11E-02
Benzene	965.2	6270.6	8912.9	7591.7	3.48E-02
2,2,4-Trimethylpentane	452.5	3661.9	4772.0	4217.0	1.94E-02
Heptane	171.2	1222.3	1635.0	1428.7	6.56E-03
Toluene	922.5	3823.0	5794.0	4808.5	2.21E-02
Octane	20.4	78.4	70.3	74.4	3.41E-04
Ethylbenzene	82.5	221.9	450.1	336.0	1.54E-03
m/p-Xylene	289.5	832.9	1723.3	1278.1	5.87E-03
Styrene	6.8	20.5	68.1	44.3	2.03E-04
o-Xylene	95.7	237.7	576.8	407.2	1.87E-03
Nonane	0.0	0.0	0.0	0.0	0.00E+00
Isopropylbenzene	0.0	0.0	0.0	0.0	0.00E+00
1,3,5 TMB	21.2	23.6	95.8	59.7	2.74E-04
Decane	0.0	0.0	0.0	0.0	0.00E+00
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	0.0	0.0	0.0	0.0	0.00E+00
Napthalene	0.0	0.0	0.0	0.0	0.00E+00
Dodecane	0.0	0.0	0.0	0.0	0.00E+00
Tridecane	2.2	0.0	0.0	0.0	0.00E+00
Biphenyl	0.0	0.0	0.0	0.0	0.00E+00
Tetradecane	0.0	0.0	0.0	0.0	0.00E+00
THC	1.32E+05	1.20E+06	1.46E+06	1.33E+06	6.10E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-3. Refueling Experiment #3: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L) Pre-fill (1)	Refueling (2) Sample	Emissions (g/gal)
Propane	250.4	939.2	4.96E-03
2-Methylpropane	15442.0	41379.1	2.18E-01
Butane	117505.8	343048.9	1.81E+00
2-Methylbutane	89543.7	243330.5	1.28E+00
1-Pentene	5760.4	15618.7	8.25E-02
2-Methyl-1-Butene	9631.3	25042.5	1.32E-01
Pentane	38868.0	98758.8	5.21E-01
Trans-2-Pentene	11301.4	29911.4	1.58E-01
Cis-2-Pentene	5974.4	15563.7	8.22E-02
2-Methyl-2-Butene	15556.6	40232.0	2.12E-01
2,2-Dimethylbutane	379.7	4928.6	2.60E-02
Cyclopentane	2370.1	5741.4	3.03E-02
MTBE	4736.5	11331.0	5.98E-02
2-Methylpentane	14523.7	35570.4	1.88E-01
3-Methylpentane	7144.2	17154.0	9.06E-02
Hexane	4821.3	10822.1	5.71E-02
Methylcyclopentane	2448.2	5591.6	2.95E-02
2,4-Dimethylpentane	708.1	1583.5	8.36E-03
Benzene	2163.7	4538.3	2.40E-02
2,2,4-Trimethylpentane	1099.8	2172.1	1.15E-02
Heptane	500.6	938.3	4.95E-03
Toluene	1566.5	2615.7	1.38E-02
Octane	62.7	93.5	4.94E-04
Ethylbenzene	133.3	199.4	1.05E-03
m/p-Xylene	492.9	772.5	4.08E-03
Styrene	21.0	32.6	1.72E-04
o-Xylene	149.2	242.9	1.28E-03
Nonane	8.5	12.6	6.66E-05
Isopropylbenzene	9.4	19.9	1.05E-04
1,3,5 TMB	35.4	56.8	3.00E-04
Decane	12.0	6.4	3.37E-05
o-Cresol	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.00E+00
Undecane	0.3	0.7	3.67E-06
Napthalene	1.4	2.2	1.14E-05
Dodecane	0.9	0.0	0.00E+00
Tridecane	0.4	0.0	0.00E+00
Biphenyl	0.0	0.0	0.00E+00
Tetradecane	0.0	0.0	0.00E+00
THC	3.93E+05	1.04E+06	5.49E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor composition during refueling

Table A-4. Refueling Experiment #4: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L) Pre-fill (1)	Refueling (2) Sample	Emissions (g/gal)
Propane	157.4	873.7	4.61E-03
2-Methylpropane	21521.8	37630.9	1.99E-01
Butane	82142.6	241648.8	1.28E+00
2-Methylbutane	78342.3	173920.9	9.18E-01
1-Pentene	4676.7	10774.1	5.69E-02
2-Methyl-1-Butene	7801.5	16938.3	8.94E-02
Pentane	34146.3	67427.4	3.56E-01
Trans-2-Pentene	9124.0	20305.3	1.07E-01
Cis-2-Pentene	4700.4	10686.5	5.64E-02
2-Methyl-2-Butene	12391.3	27173.2	1.43E-01
2,2-Dimethylbutane	287.8	3495.1	1.85E-02
Cyclopentane	1951.4	3540.2	1.87E-02
MTBE	3688.2	7215.6	3.81E-02
2-Methylpentane	12137.5	23219.2	1.23E-01
3-Methylpentane	6116.1	11283.6	5.96E-02
Hexane	4327.3	7114.9	3.76E-02
Methylcyclopentane	2050.4	3704.9	1.96E-02
2,4-Dimethylpentane	580.5	1027.5	5.43E-03
Benzene	1792.3	2889.3	1.53E-02
2,2,4-Trimethylpentane	1138.7	1456.8	7.69E-03
Heptane	424.0	614.2	3.24E-03
Toluene	1211.6	1572.8	8.30E-03
Octane	40.4	22.1	1.17E-04
Ethylbenzene	89.9	108.2	5.71E-04
m/p-Xylene	364.3	431.2	2.28E-03
Styrene	14.8	19.7	1.04E-04
o-Xylene	111.5	140.2	7.40E-04
Nonane	5.5	1.6	8.43E-06
Isopropylbenzene	7.0	9.2	4.86E-05
1,3,5 TMB	20.5	26.3	1.39E-04
Decane	4.9	3.7	1.94E-05
o-Cresol	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.00E+00
Undecane	0.6	0.8	4.48E-06
Napthalene	0.5	1.1	5.83E-06
Dodecane	1.6	0.0	0.00E+00
Tridecane	0.0	0.0	0.00E+00
Biphenyl	0.0	0.0	0.00E+00
Tetradecane	0.0	0.0	0.00E+00
THC	3.26E+05	7.31E+05	3.86E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor composition during refueling

Table A-5. Refueling Experiment #5: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	0.0	1822.8	2087.8	1955.3	1.00E-02
2-Methylpropane	1934.4	100971.5	117705.6	109338.6	5.60E-01
Butane	16524.2	502334.6	581577.8	541956.2	2.77E+00
2-Methylbutane	19110.6	345565.0	400422.7	372993.9	1.91E+00
1-Pentene	1664.5	20659.3	23406.1	22032.7	1.13E-01
2-Methyl-1-Butene	2922.7	32514.0	36965.9	34740.0	1.78E-01
Pentane	12408.3	134967.7	149643.7	142305.7	7.29E-01
Trans-2-Pentene	4557.5	39778.1	43067.0	41422.5	2.12E-01
Cis-2-Pentene	2337.6	20288.4	22041.7	21165.1	1.08E-01
2-Methyl-2-Butene	6397.0	52300.0	56714.0	54507.0	2.79E-01
2,2-Dimethylbutane	519.4	7933.4	8988.8	8461.1	4.33E-02
Cyclopentane	1159.6	7148.0	7416.4	7282.2	3.73E-02
MTBE	1808.8	14856.2	16165.4	15510.8	7.94E-02
2-Methylpentane	6811.2	49493.4	52281.0	50887.2	2.61E-01
3-Methylpentane	3578.0	24073.6	25071.0	24572.3	1.26E-01
Hexane	3249.8	14935.8	13595.5	14265.6	7.30E-02
Methylcyclopentane	1805.6	7503.8	6701.0	7102.4	3.64E-02
2,4-Dimethylpentane	479.5	2089.2	1894.9	1992.1	1.02E-02
Benzene	2129.3	4271.6	2756.6	3514.1	1.80E-02
2,2,4-Trimethylpentane	889.0	2811.0	2302.3	2556.6	1.31E-02
Heptane	548.0	1212.7	674.7	943.7	4.83E-03
Toluene	1963.2	2691.6	880.0	1785.8	9.14E-03
Octane	26.5	43.2	23.5	33.4	1.71E-04
Ethylbenzene	143.0	138.7	19.1	78.9	4.04E-04
m/p-Xylene	473.2	426.4	51.6	239.0	1.22E-03
Styrene	34.9	29.7	6.8	18.2	9.34E-05
o-Xylene	131.1	110.5	13.1	61.8	3.16E-04
Nonane	2.5	2.0	1.0	1.5	7.56E-06
Isopropylbenzene	10.0	6.6	0.0	3.3	1.69E-05
1,3,5 TMB	17.9	12.7	0.9	6.8	3.48E-05
Decane	31.6	31.2	23.1	27.2	1.39E-04
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	0.3	0.6	0.0	0.3	1.53E-06
Napthalene	8.2	7.6	6.8	7.2	3.70E-05
Dodecane	0.0	0.0	0.0	0.0	0.00E+00
Tridecane	0.0	0.0	0.0	0.0	0.00E+00
Biphenyl	0.0	0.0	0.0	0.0	0.00E+00
Tetradecane	0.0	0.0	0.0	0.0	0.00E+00
THC	1.09E+05	1.50E+06	1.68E+06	1.59E+06	8.14E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor composition during refueling

Table A-6. Refueling Experiment #6: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-fill (1)	Refueling (2)		Average	
	(ug/L)	Sample 1	Sample 2	Refueling	(g/gal)
Propane	877.8	879.0	2080.1	1479.5	7.58E-03
2-Methylpropane	33920.1	31479.2	98730.3	65104.7	3.33E-01
Butane	230685.0	212703.8	536006.0	374354.9	1.92E+00
2-Methylbutane	248241.0	228119.9	445727.8	336923.9	1.73E+00
1-Pentene	14920.7	12168.3	27897.6	20033.0	1.03E-01
2-Methyl-1-Butene	17666.1	15423.3	41160.1	28291.7	1.45E-01
Pentane	119479.0	107703.6	200134.3	153918.9	7.88E-01
Trans-2-Pentene	28871.8	24073.1	57126.1	40599.6	2.08E-01
Cis-2-Pentene	14714.6	12137.9	29299.0	20718.5	1.06E-01
2-Methyl-2-Butene	35194.4	28921.0	75716.2	52318.6	2.68E-01
2,2-Dimethylbutane	5289.1	4437.4	11317.0	7877.2	4.03E-02
Cyclopentane	5286.1	4712.1	11813.2	8262.7	4.23E-02
MTBE	10626.7	9895.9	25316.2	17606.0	9.01E-02
2-Methylpentane	32092.0	28798.6	83983.1	56390.8	2.89E-01
3-Methylpentane	15135.3	13764.9	42091.7	27928.3	1.43E-01
Hexane	9718.3	8468.3	28964.0	18716.2	9.58E-02
Methylcyclopentane	5386.8	4854.7	15943.4	10399.0	5.32E-02
2,4-Dimethylpentane	1597.4	1455.0	4742.5	3098.8	1.59E-02
Benzene	4390.2	3238.9	11741.1	7490.0	3.83E-02
2,2,4-Trimethylpentane	2531.4	2344.4	8265.0	5304.7	2.72E-02
Heptane	897.0	705.7	3460.8	2083.2	1.07E-02
Toluene	2482.2	1670.3	9770.7	5720.5	2.93E-02
Octane	92.2	47.3	408.2	227.7	1.17E-03
Ethylbenzene	110.5	57.0	608.2	332.6	1.70E-03
m/p-Xylene	295.7	142.7	1810.5	976.6	5.00E-03
Styrene	23.7	14.8	145.3	80.1	4.10E-04
o-Xylene	83.0	43.4	499.4	271.4	1.39E-03
Nonane	1.9	4.2	12.4	8.3	4.24E-05
Isopropylbenzene	4.2	0.0	0.0	0.0	0.00E+00
1,3,5 TMB	7.8	4.5	66.0	35.3	1.81E-04
Decane	2.1	5.2	6.5	5.9	3.00E-05
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	0.0	0.0	0.0	0.0	0.00E+00
Napthalene	0.8	7.8	0.0	3.9	2.01E-05
Dodecane	0.0	0.0	0.0	0.0	0.00E+00
Tridecane	0.0	0.0	0.0	0.0	0.00E+00
Biphenyl	0.0	0.0	0.0	0.0	0.00E+00
Tetradecane	0.0	0.0	0.0	0.0	0.00E+00
THC	9.07E+05	8.02E+05	1.95E+06	1.38E+06	7.05E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor composition during refueling

Table A-7. Refueling Experiment #7: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-fill (1)	Refueling (2)		Average	
		Sample1	Sample 2	Refueling	(g/gal)
Propane	579.2	756.8	685.4	721.1	3.29E-03
2-Methylpropane	29917.0	34392.8	26976.2	30684.5	1.40E-01
Butane	241399.4	256866.6	182004.9	219435.7	1.00E+00
2-Methylbutane	436436.7	516117.3	413594.1	464855.7	2.12E+00
1-Pentene	23275.3	27486.0	22085.2	24785.6	1.13E-01
2-Methyl-1-Butene	41663.3	49363.1	39391.2	44377.1	2.02E-01
Pentane	186436.1	218805.1	173734.8	196269.9	8.95E-01
Trans-2-Pentene	47775.6	55434.3	44283.8	49859.0	2.27E-01
Cis-2-Pentene	26541.0	30970.3	24366.6	27668.5	1.26E-01
2-Methyl-2-Butene	71729.5	83146.0	65909.8	74527.9	3.40E-01
2,2-Dimethylbutane	14323.7	15369.9	12042.3	13706.1	6.25E-02
Cyclopentane	10264.5	8906.4	7762.0	8334.2	3.80E-02
MTBE	42715.8	53148.2	42746.5	47947.4	2.19E-01
2-Methylpentane	89861.1	99983.4	78375.0	89179.2	4.07E-01
3-Methylpentane	46841.1	51302.0	39953.2	45627.6	2.08E-01
Hexane	27732.5	29368.6	22500.4	25934.5	1.18E-01
Methylcyclopentane	18822.2	20184.2	15794.6	17989.4	8.20E-02
2,4-Dimethylpentane	5891.1	6227.7	4904.2	5566.0	2.54E-02
Benzene	13920.6	15278.4	12275.0	13776.7	6.28E-02
2,2,4-Trimethylpentane	15267.2	15406.4	13309.2	14357.8	6.55E-02
Heptane	3728.8	3476.3	2843.0	3159.6	1.44E-02
Toluene	12892.6	11904.1	10505.7	11204.9	5.11E-02
Octane	664.6	499.1	464.0	481.5	2.20E-03
Ethylbenzene	1406.7	1023.3	947.9	985.6	4.49E-03
m/p-Xylene	5040.6	3629.4	3353.2	3491.3	1.59E-02
Styrene	377.4	215.7	219.5	217.6	9.92E-04
o-Xylene	1808.0	1261.3	1157.7	1209.5	5.52E-03
Nonane	141.3	86.2	85.7	85.9	3.92E-04
Isopropylbenzene	215.8	123.0	113.2	118.1	5.38E-04
1,3,5 TMB	431.1	343.1	299.1	321.1	1.46E-03
Decane	90.0	42.9	38.2	40.5	1.85E-04
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	68.9	4.4	2.6	3.5	1.58E-05
Napthalene	26.6	72.0	31.0	51.5	2.35E-04
Dodecane	105.6	17.0	14.5	15.7	7.17E-05
Tridecane	96.9	20.9	12.0	16.5	7.51E-05
Biphenyl	2.2	5.5	0.8	3.1	1.43E-05
Tetradecane	62.6	4.1	3.6	3.8	1.75E-05
THC	1.53E+06	1.72E+06	1.43E+06	1.58E+06	7.18E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-8. Refueling Experiment #8: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)		Emissions
	Pre-Fill (1)	Refueling (2)	(g/gal)
Propane	181.8	405.8	1.89E-03
2-Methylpropane	7811.4	16074.3	7.49E-02
Butane	52995.0	100703.4	4.69E-01
2-Methylbutane	214228.5	377451.7	1.76E+00
1-Pentene	10343.1	20643.1	9.62E-02
2-Methyl-1-Butene	18635.9	34931.9	1.63E-01
Pentane	98603.7	168385.8	7.85E-01
Trans-2-Pentene	20351.9	38990.5	1.82E-01
Cis-2-Pentene	11667.0	22143.6	1.03E-01
2-Methyl-2-Butene	30798.2	57841.0	2.70E-01
2,2-Dimethylbutane	6235.0	11067.0	5.16E-02
Cyclopentane	2642.4	4439.8	2.07E-02
MTBE	33957.4	51532.7	2.40E-01
2-Methylpentane	41254.5	71646.8	3.34E-01
3-Methylpentane	20991.1	36323.7	1.69E-01
Hexane	12403.6	20785.8	9.69E-02
Methylcyclopentane	8366.3	14503.5	6.76E-02
2,4-Dimethylpentane	2613.0	4631.0	2.16E-02
Benzene	8469.4	13393.9	6.24E-02
2,2,4-Trimethylpentane	8021.3	13072.9	6.09E-02
Heptane	1763.3	2742.3	1.28E-02
Toluene	7953.9	11532.1	5.37E-02
Octane	138.2	225.7	1.05E-03
Ethylbenzene	736.7	1034.1	4.82E-03
m/p-Xylene	2757.1	3568.5	1.66E-02
Styrene	175.8	288.0	1.34E-03
o-Xylene	1026.4	1264.8	5.89E-03
Nonane	14.7	114.1	5.32E-04
Isopropylbenzene	110.7	156.6	7.30E-04
1,3,5 TMB	364.8	405.8	1.89E-03
Decane	67.4	89.5	4.17E-04
o-Cresol	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.00E+00
Undecane	6.6	8.5	3.95E-05
Napthalene	64.9	71.2	3.32E-04
Dodecane	29.0	18.9	8.82E-05
Tridecane	4.5	16.3	7.61E-05
Biphenyl	3.7	5.7	2.65E-05
Tetradecane	3.4	5.6	2.60E-05
THC	7.10E+05	1.25E+06	5.83E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-9. Refueling Experiment #9: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-Fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	198.3	454.8	556.7	505.7	3.14E-03
2-Methylpropane	11715.4	20720.6	25153.8	22937.2	1.42E-01
Butane	76322.4	126372.2	146402.1	136387.1	8.47E-01
2-Methylbutane	292689.1	467598.3	513083.3	490340.8	3.05E+00
1-Pentene	16335.2	26618.7	29970.1	28294.4	1.76E-01
2-Methyl-1-Butene	28273.7	45619.4	50224.7	47922.1	2.98E-01
Pentane	131026.8	206037.0	222497.7	214267.3	1.33E+00
Trans-2-Pentene	32627.5	52135.5	58086.6	55111.1	3.42E-01
Cis-2-Pentene	18113.8	28693.4	31962.0	30327.7	1.88E-01
2-Methyl-2-Butene	48099.9	76971.2	84904.8	80938.0	5.03E-01
2,2-Dimethylbutane	9627.8	13707.8	14905.3	14306.6	8.88E-02
Cyclopentane	5026.7	7393.5	9182.7	8288.1	5.15E-02
MTBE	42275.7	62962.1	64134.6	63548.4	3.95E-01
2-Methylpentane	59450.9	94038.5	100687.8	97363.2	6.05E-01
3-Methylpentane	29816.8	47394.0	50418.7	48906.3	3.04E-01
Hexane	17273.1	26747.4	28194.8	27471.1	1.71E-01
Methylcyclopentane	12807.7	19760.3	21100.8	20430.5	1.27E-01
2,4-Dimethylpentane	4005.7	6160.1	6614.4	6387.3	3.97E-02
Benzene	12391.5	17992.1	19066.6	18529.4	1.15E-01
2,2,4-Trimethylpentan	12340.6	18431.8	19914.2	19173.0	1.19E-01
Heptane	2651.4	3868.0	4108.8	3988.4	2.48E-02
Toluene	12962.1	17211.3	18503.5	17857.4	1.11E-01
Octane	269.2	339.1	370.9	355.0	2.20E-03
Ethylbenzene	1454.7	1726.9	1727.1	1727.0	1.07E-02
m/p-Xylene	5207.5	6214.7	6466.3	6340.5	3.94E-02
Styrene	456.4	380.1	379.8	379.9	2.36E-03
o-Xylene	1933.9	2199.0	2268.5	2233.7	1.39E-02
Nonane	184.1	157.2	157.0	157.1	9.76E-04
Isopropylbenzene	244.0	195.3	204.4	199.8	1.24E-03
1,3,5 TMB	713.0	686.5	653.3	669.9	4.16E-03
Decane	166.4	101.1	113.0	107.0	6.65E-04
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	13.6	11.1	11.7	11.4	7.08E-05
Napthalene	145.2	134.1	105.9	120.0	7.45E-04
Dodecane	64.7	43.5	31.0	37.3	2.31E-04
Tridecane	60.6	52.4	31.8	42.1	2.61E-04
Biphenyl	5.7	15.7	8.7	12.2	7.60E-05
Tetradecane	29.4	10.5	3.9	7.2	4.49E-05
THC	1.01E+06	1.60E+06	1.72E+06	1.66E+06	1.03E+01

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-10. Refueling Experiment #10: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-Fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	365.5	477.3	432.3	454.8	2.65E-03
2-Methylpropane	16856.9	18906.6	24623.3	21764.9	1.27E-01
Butane	98130.9	109422.6	142797.4	126110.0	7.35E-01
2-Methylbutane	333188.5	358680.1	471124.6	414902.3	2.42E+00
1-Pentene	19275.1	19947.6	25690.9	22819.2	1.33E-01
2-Methyl-1-Butene	32517.3	34413.9	44915.2	39664.6	2.31E-01
Pentane	142808.5	152402.9	199458.6	175930.7	1.03E+00
Trans-2-Pentene	37545.7	39413.6	50475.0	44944.3	2.62E-01
Cis-2-Pentene	20605.1	21335.9	26642.9	23989.4	1.40E-01
2-Methyl-2-Butene	54961.1	57765.8	71590.1	64678.0	3.77E-01
2,2-Dimethylbutane	9528.3	9995.6	12771.8	11383.7	6.64E-02
Cyclopentane	5036.8	5545.2	8489.4	7017.3	4.09E-02
MTBE	42184.4	43394.8	58814.3	51104.6	2.98E-01
2-Methylpentane	64007.2	67376.5	87572.7	77474.6	4.52E-01
3-Methylpentane	31780.2	33416.3	44299.6	38857.9	2.27E-01
Hexane	17735.4	18455.3	24468.0	21461.7	1.25E-01
Methylcyclopentane	13491.6	13925.9	18548.6	16237.3	9.47E-02
2,4-Dimethylpentane	4191.6	4344.5	5763.4	5054.0	2.95E-02
Benzene	12033.6	11918.4	16569.2	14243.8	8.30E-02
2,2,4-Trimethylpentan	12592.2	12631.9	16541.4	14586.7	8.50E-02
Heptane	2580.0	2527.4	3373.6	2950.5	1.72E-02
Toluene	11834.3	10783.8	14450.9	12617.4	7.36E-02
Octane	252.3	222.6	273.9	248.3	1.45E-03
Ethylbenzene	1263.6	963.5	1249.4	1106.4	6.45E-03
m/p-Xylene	4515.1	3563.1	4598.8	4080.9	2.38E-02
Styrene	300.8	220.7	280.6	250.7	1.46E-03
o-Xylene	1612.6	1248.5	1705.7	1477.1	8.61E-03
Nonane	138.6	90.4	105.5	98.0	5.71E-04
Isopropylbenzene	163.7	112.1	117.5	114.8	6.69E-04
1,3,5 TMB	506.1	350.6	409.4	380.0	2.22E-03
Decane	640.3	715.6	3181.2	1948.4	1.14E-02
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	6.8	6.3	27.5	16.9	9.87E-05
Napthalene	78.7	42.1	46.7	44.4	2.59E-04
Dodecane	89.6	15.8	34.3	25.0	1.46E-04
Tridecane	47.4	8.5	19.7	14.1	8.21E-05
Biphenyl	3.4	35.0	0.0	17.5	1.02E-04
Tetradecane	27.7	3.5	12.0	7.8	4.53E-05
THC	1.14E+06	1.20E+06	1.56E+06	1.38E+06	8.05E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-11. Refueling Experiment #11: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-Fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	333.1	606.8	591.6	599.2	3.95E-03
2-Methylpropane	12816.3	20691.3	23901.3	22296.3	1.47E-01
Butane	70434.4	119422.8	137029.0	128225.9	8.46E-01
2-Methylbutane	242975.5	390560.9	447190.6	418875.7	2.76E+00
1-Pentene	13712.1	20808.3	23431.0	22119.7	1.46E-01
Propane	23878.1	37559.7	42738.7	40149.2	2.65E-01
2-Methylpropane	104903.7	166196.7	189581.2	177889.0	1.17E+00
Butane	27089.4	41911.9	47256.5	44584.2	2.94E-01
2-Methylbutane	15212.9	23070.0	25080.1	24075.1	1.59E-01
1-Pentene	40491.7	62839.0	68283.1	65561.0	4.33E-01
2-Methyl-1-Butene	6857.1	10749.8	11595.2	11172.5	7.37E-02
Pentane	0.0	0.0	0.0	0.0	0.00E+00
Trans-2-Pentene	34777.3	53275.1	63675.3	58475.2	3.86E-01
Cis-2-Pentene	46945.9	73111.6	82787.5	77949.6	5.14E-01
2-Methyl-2-Butene	23611.7	36578.5	42093.3	39335.9	2.60E-01
2,2-Dimethylbutane	13617.8	20617.2	23553.2	22085.2	1.46E-01
Cyclopentane	10372.5	15486.8	17640.6	16563.7	1.09E-01
MTBE	3188.0	4769.6	5416.3	5092.9	3.36E-02
2-Methylpentane	9573.4	13414.1	15868.6	14641.3	9.66E-02
3-Methylpentane	9538.5	13779.5	15517.0	14648.2	9.67E-02
Hexane	2136.4	2882.3	3253.6	3068.0	2.02E-02
Methylcyclopentane	10420.7	12528.2	13991.4	13259.8	8.75E-02
2,4-Dimethylpentane	217.6	255.6	509.1	382.3	2.52E-03
Benzene	1189.5	1182.2	1257.6	1219.9	8.05E-03
2,2,4-Trimethylpentan	3285.6	3243.7	3354.1	3298.9	2.18E-02
Heptane	291.9	267.4	332.2	299.8	1.98E-03
Toluene	1641.4	1567.4	1787.3	1677.4	1.11E-02
Octane	197.9	110.0	128.2	119.1	7.86E-04
Ethylbenzene	179.8	135.6	116.0	125.8	8.30E-04
m/p-Xylene	569.0	471.6	442.1	456.8	3.02E-03
Styrene	236.9	92.3	150.5	121.4	8.01E-04
o-Xylene	0.0	0.0	0.0	0.0	0.00E+00
Nonane	0.0	0.0	0.0	0.0	0.00E+00
Isopropylbenzene	13.6	8.0	24.6	16.3	1.08E-04
1,3,5-Trimethylbenzen	120.9	17.0	93.0	55.0	3.63E-04
Decane	95.3	23.6	39.9	31.8	2.10E-04
o-Cresol	255.9	27.9	26.0	26.9	1.78E-04
m/p-Cresol	62.0	5.2	34.0	19.6	1.29E-04
Tetradecane	143.4	13.5	11.5	12.5	8.26E-05
THC	8.50E+05	1.30E+06	1.48E+06	1.39E+06	9.17E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-12. Refueling Experiment #12: Vapor Concentration and Emissions Profile

Compound	Vapor Concentration (ug/L)				Emissions
	Pre-Fill (1)	Refueling (2)		Average	
		Sample 1	Sample 2	Refueling	(g/gal)
Propane	149.1	284.7	0.0	142.4	7.33E-04
2-Methylpropane	9098.7	14075.2	9319.7	11697.4	6.02E-02
Butane	56737.8	78977.3	55146.8	67062.0	3.45E-01
2-Methylbutane	203558.0	317889.4	324511.1	321200.3	1.65E+00
1-Pentene	10834.4	17207.7	18286.7	17747.2	9.14E-02
2-Methyl-1-Butene	19933.7	28897.5	29210.9	29054.2	1.50E-01
Pentane	89415.9	145239.1	160190.0	152714.6	7.86E-01
Trans-2-Pentene	22558.4	32704.5	34024.2	33364.4	1.72E-01
Cis-2-Pentene	12444.4	18037.8	19404.9	18721.3	9.64E-02
2-Methyl-2-Butene	34118.7	47745.7	49744.6	48745.2	2.51E-01
2,2-Dimethylbutane	5989.8	9017.3	10233.9	9625.6	4.96E-02
Cyclopentane	0.0	0.0	0.0	0.0	0.00E+00
MTBE	30938.7	58347.0	80229.4	69288.2	3.57E-01
2-Methylpentane	42521.4	63887.5	76679.7	70283.6	3.62E-01
3-Methylpentane	21621.8	32522.2	39760.5	36141.4	1.86E-01
Hexane	12613.6	21480.9	28865.5	25173.2	1.30E-01
Methylcyclopentane	9532.2	14645.9	19185.9	16915.9	8.71E-02
2,4-Dimethylpentane	2957.1	3867.9	4633.5	4250.7	2.19E-02
Benzene	9129.7	14286.7	19750.8	17018.7	8.76E-02
2,2,4-Trimethylpentane	9488.7	9586.2	10337.6	9961.9	5.13E-02
Heptane	2060.1	2612.5	3423.7	3018.1	1.55E-02
Toluene	10350.5	11582.5	15172.8	13377.6	6.89E-02
Octane	226.3	189.6	221.0	205.3	1.06E-03
Ethylbenzene	1230.7	1045.9	1244.1	1145.0	5.90E-03
m/p-Xylene	3289.4	2769.6	3179.8	2974.7	1.53E-02
Styrene	310.1	208.7	226.8	217.8	1.12E-03
o-Xylene	1631.4	1361.1	1556.5	1458.8	7.51E-03
Nonane	139.0	87.9	92.0	89.9	4.63E-04
Isopropylbenzene	188.9	253.0	346.6	299.8	1.54E-03
1,3,5 TMB	547.8	393.9	408.6	401.2	2.07E-03
Decane	220.8	216.9	428.3	322.6	1.66E-03
o-Cresol	0.0	0.0	0.0	0.0	0.00E+00
m/p-Cresol	0.0	0.0	0.0	0.0	0.00E+00
Undecane	13.5	5.4	4.4	4.9	2.53E-05
Napthalene	177.7	55.5	9.3	32.4	1.67E-04
Dodecane	29.6	13.2	11.1	12.1	6.25E-05
Tridecane	51.5	12.7	17.7	15.2	7.84E-05
Biphenyl	44.8	2.6	0.0	1.3	6.78E-06
Tetradecane	8.2	4.2	4.7	4.5	2.30E-05
THC	7.20E+05	1.07E+06	1.15E+06	1.11E+06	5.72E+00

1. Pre-fill = vapor composition prior to refueling
2. Refueling = vapor compostion during refueling

Table A-13. Austin Average Summer Refueling Vapor Concentration (ug/L)

Compound	Average	Average Weight %	Cumul.Weight %
Propane	471.5	3.38E-02	0.03
2-Methylpropane	20909.1	1.50E+00	1.53
Butane	129654.0	9.30E+00	10.83
2-Methylbutane	414604.4	2.97E+01	40.57
1-Pentene	22734.9	1.63E+00	42.20
2-Methyl-1-Butene	39349.8	2.82E+00	45.03
Pentane	180909.6	1.30E+01	58.00
Trans-2-Pentene	44475.6	3.19E+00	61.19
Cis-2-Pentene	24487.6	1.76E+00	62.95
2-Methyl-2-Butene	65381.9	4.69E+00	67.64
2,2-Dimethylbutane	11876.9	8.52E-01	68.49
Cyclopentane	4679.9	3.36E-01	68.82
MTBE	56982.7	4.09E+00	72.91
2-Methylpentane	80649.5	5.78E+00	78.70
3-Methylpentane	40865.5	2.93E+00	81.63
Hexane	23818.6	1.71E+00	83.34
Methylcyclopentane	17106.7	1.23E+00	84.56
2,4-Dimethylpentane	5163.6	3.70E-01	84.93
Benzene	15267.3	1.10E+00	86.03
2,2,4-Trimethylpentane	14300.1	1.03E+00	87.05
Heptane	3154.5	2.26E-01	87.28
Toluene	13308.2	9.55E-01	88.24
Octane	316.4	2.27E-02	88.26
Ethylbenzene	1203.0	8.63E-02	88.34
m/p-Xylene	3959.2	2.84E-01	88.63
Styrene	275.6	1.98E-02	88.65
o-Xylene	1553.6	1.11E-01	88.76
Nonane	110.7	7.94E-03	88.77
Isopropylbenzene	169.2	1.21E-02	88.78
1,3,5-Trimethylbenzene	439.1	3.15E-02	88.81
Decane	438.2	3.14E-02	88.84
o-Cresol	0.0	0.00E+00	88.84
m/p-Cresol	0.0	0.00E+00	88.84
Undecane	10.2	7.35E-04	88.84
Napthalene	62.4	4.48E-03	88.85
Dodecane	23.5	1.68E-03	88.85
Tridecane	21.8	1.57E-03	88.85
Biphenyl	9.9	7.11E-04	88.85
Tetradecane	6.9	4.95E-04	88.85
THC	1.39E+06	100	100

Table A-14. Austin Average Winter Refueling Vapor Concentration (ug/L)

Compound	Average	Average Weight %	Cumul.Weight %
Propane	1170.6	9.32E-02	0.09
2-Methylpropane	57851.7	4.61E+00	4.70
Butane	389905.2	3.10E+01	35.74
2-Methylbutane	297558.8	2.37E+01	59.43
1-Pentene	18330.5	1.46E+00	60.88
2-Methyl-1-Butene	28925.1	2.30E+00	63.19
Pentane	125116.2	9.96E+00	73.15
Trans-2-Pentene	35266.4	2.81E+00	75.96
Cis-2-Pentene	18141.6	1.44E+00	77.40
2-Methyl-2-Butene	46590.9	3.71E+00	81.11
2,2-Dimethylbutane	6423.7	5.11E-01	81.62
Cyclopentane	7157.6	5.70E-01	82.19
MTBE	13891.3	1.11E+00	83.30
2-Methylpentane	43805.9	3.49E+00	86.78
3-Methylpentane	21557.8	1.72E+00	88.50
Hexane	13696.1	1.09E+00	89.59
Methylcyclopentane	7763.7	6.18E-01	90.21
2,4-Dimethylpentane	2069.4	1.65E-01	90.37
Benzene	5592.7	4.45E-01	90.82
2,2,4-Trimethylpentane	3253.1	2.59E-01	91.08
Heptane	1226.6	9.76E-02	91.17
Toluene	3462.6	2.76E-01	91.45
Octane	91.1	7.25E-03	91.46
Ethylbenzene	220.1	1.75E-02	91.47
m/p-Xylene	796.8	6.34E-02	91.54
Styrene	37.6	2.99E-03	91.54
o-Xylene	242.2	1.93E-02	91.56
Nonane	4.0	3.18E-04	91.56
Isopropylbenzene	5.4	4.30E-04	91.56
1,3,5-Trimethylbenzene	37.8	3.01E-03	91.56
Decane	7.2	5.72E-04	91.56
o-Cresol	0.0	0.00E+00	91.56
m/p-Cresol	0.0	0.00E+00	91.56
Undecane	0.3	2.45E-05	91.56
Napthalene	2.4	1.91E-04	91.56
Dodecane	0.0	0.00E+00	91.56
Tridecane	0.6	4.58E-05	91.56
Biphenyl	0.0	0.00E+00	91.56
Tetradecane	0.3	2.44E-05	91.56
THC	1.26E+06	100	100

Table A-15. SOS (SOSVAP) and CARB (VGS710) Summer Vapor Profiles

Source: Table 2-5, Fujita, 1995b

Species	SOSVAP	VGS710
C2CMPD	0.210 ± 0.150	0.190 ± 0.180
C3CMPD	1.000 ± 0.310	2.190 ± 0.460
ETHANE	0.200 ± 0.110	0.190 ± 0.110
ETHENE	0.010 ± 0.010	0.000 ± 0.100
ACETYL	0.000 ± 0.100	0.000 ± 0.100
N_PROP	0.890 ± 0.310	2.190 ± 0.450
PROPE	0.110 ± 0.010	0.000 ± 0.100
I_BUTA	4.830 ± 0.430	11.510 ± 2.300
BEABYL	0.900 ± 0.480	0.000 ± 0.100
N_BUTA	20.860 ± 3.020	30.220 ± 6.050
T2BUTE	1.490 ± 0.520	1.690 ± 0.350
C2BUTE	1.370 ± 0.480	1.350 ± 0.290
B1E3ME	0.520 ± 0.100	0.420 ± 0.130
IPENTA	28.040 ± 0.730	22.400 ± 4.480
PENTE1	1.210 ± 0.260	1.010 ± 0.230
N_PENT	7.510 ± 2.290	6.320 ± 1.270
I_PREN	0.070 ± 0.010	0.000 ± 0.100
T2PENE	2.350 ± 0.490	1.680 ± 0.350
C2PENE	1.280 ± 0.270	0.850 ± 0.200
B2E2M	3.240 ± 0.630	0.000 ± 0.100
BU22DM	0.720 ± 0.240	1.060 ± 0.230
CPENTE	0.390 ± 0.060	0.000 ± 0.100
P1E4ME	0.250 ± 0.050	0.000 ± 0.100
CPENTA	0.450 ± 0.130	0.510 ± 0.140
PENA3M	2.100 ± 0.400	1.560 ± 0.330
PENA2M	3.810 ± 0.770	2.330 ± 0.480
BU23DM	1.620 ± 0.580	0.720 ± 0.180
P1E2ME	0.290 ± 0.020	0.000 ± 0.100
N_HEX	1.300 ± 0.270	1.140 ± 0.250
T2HEXE	0.320 ± 0.070	0.000 ± 0.100
C2HEXE	0.180 ± 0.040	0.000 ± 0.100
MCYPNA	0.900 ± 0.200	1.080 ± 0.240
PEN24M	0.660 ± 0.320	0.400 ± 0.130
BENZE	0.970 ± 0.060	0.590 ± 0.150
CYHEXA	0.130 ± 0.040	0.330 ± 0.120
HEXA2M	0.570 ± 0.060	0.410 ± 0.130
PEN23M	0.650 ± 0.380	0.330 ± 0.120
HEXA3M	0.550 ± 0.040	0.330 ± 0.120
PA224M	1.560 ± 1.460	0.000 ± 0.100
N_HEPT	0.280 ± 0.010	0.220 ± 0.110
MECYHX	0.130 ± 0.020	0.090 ± 0.100
PA234M	0.420 ± 0.340	0.000 ± 0.100
TOLUE	1.930 ± 1.000	0.570 ± 0.150

Table A-15. SOS (SOSVAP) and CARB (VGS710) Summer Vapor Profiles

Source: Table 2-5, Fujita, 1995b

Species	SOSVAP	VGS710
HEP2ME	0.090 ± 0.010	0.000 ± 0.100
HEP3ME	0.030 ± 0.060	0.000 ± 0.100
N_OCT	0.060 ± 0.030	0.020 ± 0.100
ETBZ	0.200 ± 0.080	0.030 ± 0.100
MP_XYL	0.620 ± 0.270	0.110 ± 0.100
STYR	0.020 ± 0.100	0.000 ± 0.100
O_XYL	0.220 ± 0.090	0.040 ± 0.100
N_NON	0.020 ± 0.100	0.000 ± 0.100
IPRBZ	0.030 ± 0.010	0.000 ± 0.100
N_PRBZ	0.040 ± 0.010	0.000 ± 0.100
BZ135M	0.060 ± 0.010	0.000 ± 0.100
BZ124M	0.180 ± 0.030	0.310 ± 0.120
UNID	3.370 ± 6.590	7.990 ± 11.500

Table A-16. Austin Measured and Predicted, CARB, and SOS Gasoline Vapor Summer Speciation Profile Comparison

	Concentration, % by weight			
Compound	Austin, Measured	Austin, Predicted	SOSVAP	VGS710
iso-Butane	1.5	1.8	4.8	11.5
Butane	9.3	7.6	20.9	30.2
iso-Pentane	29.7	24.5	28.0	22.4
Pentene	1.6	1.3	1.2	1.0
Pentane	13.0	10.5	7.5	6.3
trans-2-Pentene	3.2	2.6	2.4	1.7
cis-2-Pentene	1.8	1.4	1.3	0.9
2,2, Dimethylbutane	0.9	0.7	0.7	1.1
Cyclopentane	0.3	0.5	0.4	0.5
3-Methylpentane	2.9	2.2	2.1	1.6
2-Methylpentane	5.8	3.9	3.8	2.3
Hexane	1.7	1.3	1.3	1.1
Methylcyclopentane	1.2	0.9	0.9	1.1
Benzene	1.1	0.7	1.0	0.6
2,2,4-TMP	1.0	0.7	1.6	0.0
Heptane	0.2	0.1	0.3	0.2
Toluene	1.0	0.6	1.9	0.6
Octane	0.0	0.0	0.1	0.0
Ethylbenzene	0.1	0.1	0.2	0.0
m,p-Xylene	0.3	0.2	0.6	0.1
Styrene	0.0	0.0	0.0	0.0
o-Xylene	0.1	0.1	0.2	0.0
Nonane	0.0	0.0	0.0	0.0
Cumene	0.0	0.0	0.0	0.0
1,3,5-TMB	0.0	0.0	0.1	0.0
Total	76.7	61.8	81.3	83.2

Table A-17. Predicted vs Measured Total VOC Emissions

					Total VOC Emissions (g VOC/gallon gasoline)		
Experiment	T_d (°F)	T_t (°F)	ΔT (°F)	RVP	Measured	AP-42	ORVR
1	63	75	12	12.7	6.78	4.68	5.00
2	63	75	12	12.7	6.13	4.68	5.00
3	73.8	78.8	5	11	5.50	5.48	5.16
4	7.38	78.8	5	11	3.86	5.48	5.16
5	73	80	7	11.4	8.14	5.41	5.30
6	73	80	7	11.4	7.06	5.41	5.30
7	91.1	94.7	3.6	9.6	7.17	6.46	6.14
8	91.1	94.7	3.6	9.3	5.84	6.31	5.90
9	85.7	94.7	9	8.4	10.4	4.89	4.57
10	85.7	84.6	-1.1	9.5	8.02	6.38	5.55
11	91.1	94.7	3.6	10	9.19	6.65	6.47
12	85.7	85.7	0	8.15	5.72	5.62	4.63
Exp 1-12 ave					6.98	5.62	5.35
Exp 7-12 ave					7.72	6.05	5.54

APPENDIX B - TEVAP SPECIATION MODEL

TEVAP Model Overview

The purpose of the TEVAP Model is to speciation profiles for the three following categories of evaporative emissions:

- running loss
- hot soak
- diurnal

For each emission category, speciation profiles are developed using vapor- and/or liquid-based evaporative emissions data. Speciation profiles are provided as compound-specific profiles, expressed in units of percent by mass

The TEVAP Model is a spreadsheet model and has the following spreadsheet pages:

- input
- output
- compound data
- speciation calculations, one for each emission category

A brief description of each page is provided below.

Input

The input portion of this page contains information that is required for model execution. User supplied data consists of diurnal range minimum and maximum temperature values in degrees Fahrenheit, gasoline Reid vapor pressure (RVP) and liquid speciation data e.g., compound-specific percent by mass composition data. The model currently accepts speciation data information on a total of 197 individual compounds. A list of these compounds and the data required for use by the TEVAP Model, e.g., molecular weight and boiling point, is provided.

The user selects emission source categories for which speciation profiles are to be calculated.

Temperatures used to calculate hot soak, running loss, and diurnal emissions are calculated as follows:

Temperature for diurnal loss emissions
= (maximum hourly temp + minimum hourly temp)/2

Temperature for hot soak and running loss emissions
= 2/3(maximum hourly temp) + 1/3(minimum hourly temp)

where all temperatures are expressed in degrees Fahrenheit.

Output

The output page contains speciation profiles for each of the three emission source categories. Speciation profiles are provided as compound-specific profiles, expressed in units of percent by mass.

Compound Data

The compound data page contains molecular weight and boiling point data for all compounds included in the model.

Speciation Calculation

There are three individual speciation pages, one for each emissions category. Based on user input data, the speciation calculation page calculates a vapor-based speciation profile. Speciation profiles are calculated using the following algorithms:

1. Calculation of gasoline vapor pressure (Gas VP):

$$\text{Gas VP (psia)} = \exp[(0.7553 - 413/\text{TEMP}) * 3^{0.5} * \text{LOG(RVP)} - (1{,}854 - 1042/\text{TEMP}) * 3^{0.5} + (2416/\text{TEMP} - 2.013) * \text{LOG(RVP)} - 8742/\text{TEMP} + 15.64]$$

where:

TEMP = temperature of concern, deg F; and
RVP = gasoline Reid vapor pressure, (psia).

Algorithm source: Shedd, S.A. "Gasoline Marketing", In Air Pollution Engineering Manual, Buonicore, A.J.; Davis, W.T., Eds.; Van Nostrand Reinhold: New York, 1992 p. 341.

2. Calculation of liquid gasoline molecular weight (Liq MW):

$$\text{Liq MW} = -0.7695 * \text{RVP} + 97.24$$

Algorithm source: Data used for development of the Liq MW algorithm was obtained from API Publication 4534, Effects of fuel RVP and Fuel Blends on Emissions at Non-FTP Temperatures, Volume II: Compilation of Test Data and Laboratory Procedures, June 1991.

3. Calculation of gasoline vapor molecular weight (Vap MW):

$$\text{Vap MW} = 72.833 - 1.3183 * \text{RVP} + 0.15079 * \text{RVP}^2 - 0.0087302 * \text{RVP}^3$$

Algorithm source: Shedd, S.A. "Gasoline Marketing", In Air Pollution Engineering Manual, Buonicore, A.J.; Davis, W.T., Eds.; Van Nostrand Reinhold: New York, 1992 p. 341.

4. Calculation of Gas Mr:

$$\text{Gas Mr} = (\text{Vap MW} + MW_{air}) / (\text{Vap MW} * MW_{air})$$

where:

MW_{air} = molecular weight of air, g/gmol.

Algorithm source: Lyman, W. J., Reehl, W. F., and D. H. Rosenblatt, Handbook of Chemical Property Estimation Methods, p. 17-6, American Chemical Society, Washington, DC, 1990.

5. Calculation of compound-specific vapor pressure (Cmpd VP, psia):

$$\text{Cmpd VP} = [\exp(19 * (1 - \text{BP/TEMP}) + 8.5 * \ln(\text{BP/TEMP}))] * 14.7$$

where:

BP = compound specific boiling point, deg K.

Algorithm source: Schwarzenbach, R. P., Gschwend, P. M., and D. M. Imboden, Environmental Organic Chemistry, p. 73, John Wiley & Sons, New York, 1993.

6. Calculation of compound-specific liquid mole fraction (Liq MOL FRAC):

$$\text{Liq MOL FRAC} = (\text{Liq Comp / Cmpd MW}) * (100/\text{Liq MW})$$

where:

Liq comp = user defined compound liquid composition, percent by mass; and
Cmpd = compound-specific molecular weight, g/gmol.

7. Calculation of compound-specific partial pressure, (Cmpd Pp, psia):

$$\text{Cmpd Pp} = \text{Cmpd VP} * \text{Liq MOL FRAC}$$

8. Calculation of compound-specific Mr, (Cmpd Mr):

$$\text{Cmpd Mr} = (\text{Cmpd MW} + MW_{air}) / (\text{Cmpd MW} * MW_{air})$$

9. Calculation of compound-specific vapor mole fraction (Vap MOL FRAC):

$$\text{Vap MOL FRAC} = (\text{Cmpd Pp/Gas VP}) * (\text{Cmpd Mr/Gas Mr})^{0.5}$$

10. Calculation of compound-specific speciation profile, (Vap SPEC, % by mass):

Vap SPEC = Vap MOL FRAC * Adj. Factor * (Cmpd MW/Vap MW) * 100

where:

Adj. Factor = user-defined model adjustment factor, model default, Adj. Factor = 1.

User Input Page **p. 1 of 4**

Selection of Emissions Categories

Calculate Hot Soak emissions	1	(Enter 1 to perform, 0 to omit)
Calculate Diurnal emissions	1	(Enter 1 to perform, 0 to omit)
Calculate Running Loss emissions	1	(Enter 1 to perform, 0 to omit)

Selection of Emissions "Bins"

Vapor-based "regular-emitter" category

Calculate Hot Soak Regular-emitter emissions	1	(Enter 1 to perform, 0 to omit)
Calculate Diurnal Regular-emitter emissions	1	(Enter 1 to perform, 0 to omit)
Calculate Running Loss Regular-emitter emissions	1	(Enter 1 to perform, 0 to omit)

Gasoline Data

RVP (psia)	7	
Diurnal minimum temperature (deg F)	105	
Diurnal maximum temperature (deg F)	105	
Hot Soak ambient temperature (deg F)	105	(calculated, 2/3*max + 1/3*min)
Diurnal average temperature (deg F)	105	(calculated, (max + min)/2)
Running Loss ambient temperature (deg F)	105	(calculated, 2/3*max + 1/3*min)

Liquid Composition

Compound	(% by mass)
PARAFFINS	
Methane	0
Ethane	0
Propane	0
Butane	0.22
n-Pentane	4.01
n-Hexane	1.8
n-Heptane	1.21
n-Octane	0.73
n-Nonane	0.22
n-Decane	0.14
n-Undecane	0.12
n-Dodecane	0.09
n-Tridecane	0
n-Tetradecane	0
n-Pentadecane	0
ISOPARAFFINS	
Isobutane	0.05
2,2-dimethylpropane	0
Isopentane	8.89
2,3-Dimethylbutane	1.98
2-Methylpentane	3.97
3-Methylpentane	2.19
2,2-Dimethylpentane	0.08
2,4-Dimethylpentane	0.41
2,2,3-Trimethylbutane	0.03
3,3-Dimethylpentane	0.08
2-Methylhexane	1.59
2,3-Dimethylpentane	0.27
3-Methylhexane	1.4
3-Ethylpentane	

2,2-Dimethylhexane	0.27
2,5-Dimethylhexane	0.16
2,2,3-Trimethylpentane	
2,4-Dimethylhexane	0.51
2,3-Dimethylhexane	0.29
2-Methylheptane	0.65
4-Methylheptane	0.37
3-Methylheptane	0.87
3-Ethylhexane	
2,5-Dimethylheptane	
3,5-Dimethylheptane (D)	0.37
3,3-Dimethylheptane	
3,5-Dimethylheptane (L)	
2,3-Dimethylheptane	0.05
3,4-Dimethylheptane (D)	
3,4-Dimethylheptane (L)	
2-Methyloctane	0
3-Methyloctane	0.38
3,3-Diethylpentane	
2,2-Dimethyloctane	0.06
3,3-Dimethyloctane	
2,3-Dimethyloctane	
2-Methylnonane	
3-Ethyloctane	
3-Methylnonane	0
2,2-dimethylbutane	0.44
2,2,4-TriMePentane	0.61
3,3-Dimethylhexane	0.19
2,3,4-Trimethylpentane	0.48
2,3-MethylEthylPentane	
2,3,5-trimethylhexane	0.05
2,4-Dimethylheptane	0.17
4-Methyloctane	0.48

AROMATICS

Benzene	1.42
Toluene	7.17
Ethylbenzene	1.04
m-Xylene	3.34
p-Xylene	0
o-Xylene	1.41
Isopropylbenzene	0.1
n-Propylbenzene	0.52
1-Methyl-3-Ethylbenzene	1.81
1-Methyl-4-Ethylbenzene	0.81
1,3,5-Trimethylbenzene	0.94
1-Methyl-2-Ethylbenzene	
1,2,4-Trimethylbenzene	2.72
tert-Butylbenzene	0
Isobutylbenzene	0.06
sec-Butylbenzene	0.06
1-Methyl-3-Isopropylbenzene	
1-Methyl-4-Isopropylbenzene	0.07
1-Methyl-2-Isopropylbenzene	
1-Methyl-3-n-Propylbenzene	0.44
1-Methyl-4-n-Propylbenzene	0.04
n-Butylbenzene	0.07
1,3-Dimethyl-5-Ethylbenzene	
1,2-Diethylbenzene	0.06
1-Methyl-2-n-Propylbenzene	0.21
1,4-Dimethyl-2-Ethylbenzene	0.39
1,2-Dimethyl-4-Ethylbenzene	0.48

1,3-Dimethyl-2-Ethylbenzene	0.25
1,2-Dimethyl-3-Ethylbenzene	
1,2,4,5-Tetramethylbenzene	0.26
2-Methylbutylbenzene	
tert-1-Butyl-2-Methylbenzene	
n-Pentylbenzene	
t-1-Butyl-3,5-Dimethylbenzene	
t-1-Butyl-4-Ethylbenzene	
1,3,5-Triethylbenzene	
1,2,4-Triethylbenzene	
n-Hexylbenzene	
1,2,3-TrimethylBenzene	0.67
1,3-Diethylbenzene	0.22
1,4-Diethylbenzene	0.85
1,2,3,5-Tetramethylbenzene	0.39
1,2,3,4-Tetramethylbenzene	0.18
Amylbenzene	0
1,4-Diisopropylbenzene	0.01
Naphthalene	0.39
NAPTHENES	
Cyclopentane	0
Methylcyclopentane	1.68
Cyclohexane	0.52
1,1-Dimethylcyclopentane	
cis-1,3-Dimethylcyclopentane	0.42
trans-1,3-Dimethylcyclopentane	
trans-1,2-Dimethylcyclopentane	0.71
Methylcyclohexane	0.84
Ethylcyclopentane	0
ctc-1,2,4-Trimethylcyclopentane	
ctc-1,2,3-Trimethylcyclopentane	0
cct-1,2,4-Trimethylcyclopentane	
trans-1,4-Dimethylcyclohexane	0.07
1-Ethyl-1-Methylcyclopentane	
trans-1,2-Dimethylcyclohexane	0.17
ccc-1,2,3-Trimethylcyclopentane	
Isopropylcyclopentane	
cis-1,2-Dimethylcyclohexane	0.06
n-Propylcyclopentane	
ccc-1,3,5-Trimethylcyclohexane	
1,1,4-Trimethylcyclohexane	
ctt-1,2,4-Trimethylcyclohexane	
ctc-1,2,4-Trimethylcyclohexane	
1,1,2-Trimethylcyclohexane	
Isobutylcyclopentane	
Isopropylcyclohexane	
n-Butylcyclopentane	
Isobutylcyclohexane	
t-1-Methyl-2-Propylcyclohexane	
t-1-Methyl-2-(4MP)cyclopentane	
cis-1,3-Dimethylcyclohexane	0.26
2,2,5-Trimethylhexane	0.15
1,1-Dimethylcyclohexane	0.25
Ethylcyclohexane	0.07
c-1,4-Dimethylcyclohexane	0.29
OLEFINS	
Isobutene	0.04
1-Butene	0
cis-2-Butene	0.14
3-Methyl-1-Butene	0.08

1-Pentene	0.25
2-Methyl-1-Butene	0.22
2-Methyl-1,3-Butadiene	0.02
trans-2-Pentene	1.62
cis-2-Pentene	0.75
4-Methylpentene-1	0.25
1-Hexene	0.77
trans-2-Hexene	0.85
2-Methylpentene-2	0.66
cis-2-Hexene	0.54
1-Heptene	0.12
trans-3-Heptene	0.32
cis-3-Heptene	0.88
trans-2-Heptene	0.28
cis-2-Heptene	0.43
1-Octene	0
trans-2-Octene	
cis-2-Octene	0.06
1-Nonene	0.2
trans-3-Nonene	
cis-3-Nonene	
trans-2-Nonene	
cis-2-Nonene	0.06
1-Decene	
2-methylpropene	0
t-2-butene	0.19
2-methyl-2-butene	0.86
cyclopentadiene	0.02
cyclopentene	0.32
3-methyl-1-pentene	0
4-Me-c-2-Pentene	0
2-methyl-1-pentene	0
c-3-hexene	0.33
3-MeCyclopentene	0
1-methylcyclopentene	0.75
3-Me-1-Hexene	0.14
2-Methyl-2-hexene	
3-ethyl-c-2-pentene	0.1
2,3-DMe-2-Pentene	0.25
2,4,4-Trimethyl-2-Pentene	0.09
1-MethylCycloHexene	
1-Undecene	0.04
1-Dodecene	0.16
OXYGENATE	
MTBE	6.35
ETBE	0
OTHER	
Ethyne	0
Propyne	
Propadiene	0
Indan	0.51
Cyclohexene	0
TOTAL	**86.4**

ATL identified and quantified	91.01
Percentage ofATL-identified cmpds included in analysis	**94.9**

Compound	Speciation profile (% by mass) Hot Soak	Diurnal	Running Loss
PARAFFINS			
Methane	0.000E+00	0.000E+00	0.000E+00
Ethane	0.000E+00	0.000E+00	0.000E+00
Propane	0.000E+00	0.000E+00	0.000E+00
Butane	2.018E+00	2.018E+00	2.018E+00
n-Pentane	1.132E+01	1.132E+01	1.132E+01
n-Hexane	1.610E+00	1.610E+00	1.610E+00
n-Heptane	3.567E-01	3.567E-01	3.567E-01
n-Octane	7.439E-02	7.439E-02	7.439E-02
n-Nonane	8.128E-03	8.128E-03	8.128E-03
n-Decane	1.967E-03	1.967E-03	1.967E-03
n-Undecane	6.698E-04	6.698E-04	6.698E-04
n-Dodecane	2.084E-04	2.084E-04	2.084E-04
n-Tridecane	0.000E+00	0.000E+00	0.000E+00
n-Tetradecane	0.000E+00	0.000E+00	0.000E+00
n-Pentadecane	0.000E+00	0.000E+00	0.000E+00
ISOPARAFFINS			
Isobutane	6.330E-01	6.330E-01	6.330E-01
2,2-dimethylpropane	0.000E+00	0.000E+00	0.000E+00
Isopentane	3.285E+01	3.285E+01	3.285E+01
2,3-Dimethylbutane	2.589E+00	2.589E+00	2.589E+00
2-Methylpentane	4.792E+00	4.792E+00	4.792E+00
3-Methylpentane	2.378E+00	2.378E+00	2.378E+00
2,2-Dimethylpentane	4.815E-02	4.815E-02	4.815E-02
2,4-Dimethylpentane	2.353E-01	2.353E-01	2.353E-01
2,2,3-Trimethylbutane	1.698E-02	1.698E-02	1.698E-02
3,3-Dimethylpentane	3.742E-02	3.742E-02	3.742E-02
2-Methylhexane	6.415E-01	6.415E-01	6.415E-01
2,3-Dimethylpentane	1.039E-01	1.039E-01	1.039E-01
3-Methylhexane	5.283E-01	5.283E-01	5.283E-01
3-Ethylpentane	0.000E+00	0.000E+00	0.000E+00
2,2-Dimethylhexane	5.707E-02	5.707E-02	5.707E-02
2,5-Dimethylhexane	3.101E-02	3.101E-02	3.101E-02
2,2,3-Trimethylpentane	0.000E+00	0.000E+00	0.000E+00
2,4-Dimethylhexane	9.763E-02	9.763E-02	9.763E-02
2,3-Dimethylhexane	4.375E-02	4.375E-02	4.375E-02
2-Methylheptane	9.179E-02	9.179E-02	9.179E-02
4-Methylheptane	5.144E-02	5.144E-02	5.144E-02
3-Methylheptane	1.196E-01	1.196E-01	1.196E-01
3-Ethylhexane	0.000E+00	0.000E+00	0.000E+00
2,5-Dimethylheptane	0.000E+00	0.000E+00	0.000E+00
3,5-Dimethylheptane (D)	2.478E-02	2.478E-02	2.478E-02
3,3-Dimethylheptane	0.000E+00	0.000E+00	0.000E+00
3,5-Dimethylheptane (L)	0.000E+00	0.000E+00	0.000E+00
2,3-Dimethylheptane	2.798E-03	2.798E-03	2.798E-03
3,4-Dimethylheptane (D)	0.000E+00	0.000E+00	0.000E+00
3,4-Dimethylheptane (L)	0.000E+00	0.000E+00	0.000E+00
2-Methyloctane	0.000E+00	0.000E+00	0.000E+00
3-Methyloctane	1.885E-02	1.885E-02	1.885E-02
3,3-Diethylpentane	0.000E+00	0.000E+00	0.000E+00
2,2-Dimethyloctane	1.715E-03	1.715E-03	1.715E-03
3,3-Dimethyloctane	0.000E+00	0.000E+00	0.000E+00
2,3-Dimethyloctane	0.000E+00	0.000E+00	0.000E+00
2-Methylnonane	0.000E+00	0.000E+00	0.000E+00
3-Ethyloctane	0.000E+00	0.000E+00	0.000E+00
3-Methylnonane	0.000E+00	0.000E+00	0.000E+00
2,2-dimethylbutane	7.660E-01	7.660E-01	7.660E-01
2,2,4-TriMePentane	1.724E-01	1.724E-01	1.724E-01
3,3-Dimethylhexane	3.295E-02	3.295E-02	3.295E-02
2,3,4-Trimethylpentane	8.009E-02	8.009E-02	8.009E-02
2,3-MethylEthylPentane	0.000E+00	0.000E+00	0.000E+00
2,3,5-trimethylhexane	4.083E-03	4.083E-03	4.083E-03
2,4-Dimethylheptane	1.283E-02	1.283E-02	1.283E-02
4-Methyloctane	2.529E-02	2.529E-02	2.529E-02

	Speciation profile (% by mass)		
	Hot Soak	Diurnal	Running Loss
AROMATICS			
Benzene	8.532E-01	8.532E-01	8.532E-01
Toluene	1.342E+00	1.342E+00	1.342E+00
Ethylbenzene	7.043E-02	7.043E-02	7.043E-02
m-Xylene	2.014E-01	2.014E-01	2.014E-01
p-Xylene	0.000E+00	0.000E+00	0.000E+00
o-Xylene	6.870E-02	6.870E-02	6.870E-02
Isopropylbenzene	3.485E-03	3.485E-03	3.485E-03
n-Propylbenzene	1.372E-02	1.372E-02	1.372E-02
1-Methyl-3-Ethylbenzene	4.385E-02	4.385E-02	4.385E-02
1-Methyl-4-Ethylbenzene	1.908E-02	1.908E-02	1.908E-02
1,3,5-Trimethylbenzene	1.979E-02	1.979E-02	1.979E-02
1-Methyl-2-Ethylbenzene	0.000E+00	0.000E+00	0.000E+00
1,2,4-Trimethylbenzene	4.730E-02	4.730E-02	4.730E-02
tert-Butylbenzene	0.000E+00	0.000E+00	0.000E+00
Isobutylbenzene	8.967E-04	8.967E-04	8.967E-04
sec-Butylbenzene	8.766E-04	8.766E-04	8.766E-04
1-Methyl-3-Isopropylbenzene	0.000E+00	0.000E+00	0.000E+00
1-Methyl-4-Isopropylbenzene	8.731E-04	8.731E-04	8.731E-04
1-Methyl-2-Isopropylbenzene	0.000E+00	0.000E+00	0.000E+00
1-Methyl-3-n-Propylbenzene	4.469E-03	4.469E-03	4.469E-03
1-Methyl-4-n-Propylbenzene	3.830E-04	3.830E-04	3.830E-04
n-Butylbenzene	6.744E-04	6.744E-04	6.744E-04
1,3-Dimethyl-5-Ethylbenzene	0.000E+00	0.000E+00	0.000E+00
1,2-Diethylbenzene	5.744E-04	5.744E-04	5.744E-04
1-Methyl-2-n-Propylbenzene	1.884E-03	1.884E-03	1.884E-03
1,4-Dimethyl-2-Ethylbenzene	3.236E-03	3.236E-03	3.236E-03
1,2-Dimethyl-4-Ethylbenzene	3.561E-03	3.561E-03	3.561E-03
1,3-Dimethyl-2-Ethylbenzene	1.814E-03	1.814E-03	1.814E-03
1,2-Dimethyl-3-Ethylbenzene	0.000E+00	0.000E+00	0.000E+00
1,2,4,5-Tetramethylbenzene	1.415E-03	1.415E-03	1.415E-03
2-Methylbutylbenzene	0.000E+00	0.000E+00	0.000E+00
tert-1-Butyl-2-Methylbenzene	0.000E+00	0.000E+00	0.000E+00
n-Pentylbenzene	0.000E+00	0.000E+00	0.000E+00
t-1-Butyl-3,5-Dimethylbenzene	0.000E+00	0.000E+00	0.000E+00
t-1-Butyl-4-Ethylbenzene	0.000E+00	0.000E+00	0.000E+00
1,3,5-Triethylbenzene	0.000E+00	0.000E+00	0.000E+00
1,2,4-Triethylbenzene	0.000E+00	0.000E+00	0.000E+00
n-Hexylbenzene	0.000E+00	0.000E+00	0.000E+00
1,2,3-TrimethylBenzene	9.214E-03	9.214E-03	9.214E-03
1,3-Diethylbenzene	2.331E-03	2.331E-03	2.331E-03
1,4-Diethylbenzene	7.942E-03	7.942E-03	7.942E-03
1,2,3,5-Tetramethylbenzene	2.025E-03	2.025E-03	2.025E-03
1,2,3,4-Tetramethylbenzene	6.902E-04	6.902E-04	6.902E-04
Amylbenzene	0.000E+00	0.000E+00	0.000E+00
1,4-Diisopropylbenzene	4.113E-05	4.113E-05	4.113E-05
Naphthalene	8.581E-04	8.581E-04	8.581E-04

	Speciation profile (% by mass)		
	Hot Soak	Diurnal	Running Loss
NAPTHENES			
Cyclopentane	0.000E+00	0.000E+00	0.000E+00
Methylcyclopentane	1.350E+00	1.350E+00	1.350E+00
Cyclohexane	3.024E-01	3.024E-01	3.024E-01
1,1-Dimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
cis-1,3-Dimethylcyclopentane	1.654E-01	1.654E-01	1.654E-01
trans-1,3-Dimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
trans-1,2-Dimethylcyclopentane	2.685E-01	2.685E-01	2.685E-01
Methylcyclohexane	2.720E-01	2.720E-01	2.720E-01
Ethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
ctc-1,2,4-Trimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
ctc-1,2,3-Trimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
cct-1,2,4-Trimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
trans-1,4-Dimethylcyclohexane	9.128E-03	9.128E-03	9.128E-03
1-Ethyl-1-Methylcyclopentane	0.000E+00	0.000E+00	0.000E+00
trans-1,2-Dimethylcyclohexane	1.896E-02	1.896E-02	1.896E-02
ccc-1,2,3-Trimethylcyclopentane	0.000E+00	0.000E+00	0.000E+00
Isopropylcyclopentane	0.000E+00	0.000E+00	0.000E+00
cis-1,2-Dimethylcyclohexane	5.220E-03	5.220E-03	5.220E-03
n-Propylcyclopentane	0.000E+00	0.000E+00	0.000E+00
ccc-1,3,5-Trimethylcyclohexane	0.000E+00	0.000E+00	0.000E+00
1,1,4-Trimethylcyclohexane	0.000E+00	0.000E+00	0.000E+00
ctt-1,2,4-Trimethylcyclohexane	0.000E+00	0.000E+00	0.000E+00
ctc-1,2,4-Trimethylcyclohexane	0.000E+00	0.000E+00	0.000E+00
1,1,2-Trimethylcyclohexane	0.000E+00	0.000E+00	0.000E+00
Isobutylcyclopentane	0.000E+00	0.000E+00	0.000E+00
Isopropylcyclohexane	0.000E+00	0.000E+00	0.000E+00
n-Butylcyclopentane	0.000E+00	0.000E+00	0.000E+00
Isobutylcyclohexane	0.000E+00	0.000E+00	0.000E+00
t-1-Methyl-2-Propylcyclohexane	0.000E+00	0.000E+00	0.000E+00
t-1-Methyl-2-(4MP)cyclopentane	0.000E+00	0.000E+00	0.000E+00
cis-1,3-Dimethylcyclohexane	3.313E-02	3.313E-02	3.313E-02
2,2,5-Trimethylhexane	1.614E-02	1.614E-02	1.614E-02
1,1-Dimethylcyclohexane	3.186E-02	3.186E-02	3.186E-02
Ethylcyclohexane	5.566E-03	5.566E-03	5.566E-03
c-1,4-Dimethylcyclohexane	3.695E-02	3.695E-02	3.695E-02

	Speciation profile (% by mass)		
	Hot Soak	Diurnal	Running Loss
OLEFINS			
Isobutene	4.445E-01	4.445E-01	4.445E-01
1-Butene	0.000E+00	0.000E+00	0.000E+00
cis-2-Butene	1.140E+00	1.140E+00	1.140E+00
3-Methyl-1-Butene	3.805E-01	3.805E-01	3.805E-01
1-Pentene	8.655E-01	8.655E-01	8.655E-01
2-Methyl-1-Butene	7.325E-01	7.325E-01	7.325E-01
2-Methyl-1,3-Butadiene	6.068E-02	6.068E-02	6.068E-02
trans-2-Pentene	4.547E+00	4.547E+00	4.547E+00
cis-2-Pentene	2.064E+00	2.064E+00	2.064E+00
4-Methylpentene-1	3.782E-01	3.782E-01	3.782E-01
1-Hexene	8.323E-01	8.323E-01	8.323E-01
trans-2-Hexene	7.859E-01	7.859E-01	7.859E-01
2-Methylpentene-2	6.229E-01	6.229E-01	6.229E-01
cis-2-Hexene	4.817E-01	4.817E-01	4.817E-01
1-Heptene	4.247E-02	4.247E-02	4.247E-02
trans-3-Heptene	1.049E-01	1.049E-01	1.049E-01
cis-3-Heptene	2.878E-01	2.878E-01	2.878E-01
trans-2-Heptene	8.429E-02	8.429E-02	8.429E-02
cis-2-Heptene	1.272E-01	1.272E-01	1.272E-01
1-Octene	0.000E+00	0.000E+00	0.000E+00
trans-2-Octene	0.000E+00	0.000E+00	0.000E+00
cis-2-Octene	6.138E-03	6.138E-03	6.138E-03
1-Nonene	8.669E-03	8.669E-03	8.669E-03
trans-3-Nonene	0.000E+00	0.000E+00	0.000E+00
cis-3-Nonene	0.000E+00	0.000E+00	0.000E+00
trans-2-Nonene	0.000E+00	0.000E+00	0.000E+00
cis-2-Nonene	2.437E-03	2.437E-03	2.437E-03
1-Decene	0.000E+00	0.000E+00	0.000E+00
2-methylpropene	0.000E+00	0.000E+00	0.000E+00
t-2-butene	1.547E+00	1.547E+00	1.547E+00
2-methyl-2-butene	2.211E+00	2.211E+00	2.211E+00
cyclopentadiene	4.691E-02	4.691E-02	4.691E-02
cyclopentene	6.985E-01	6.985E-01	6.985E-01
3-methyl-1-pentene	0.000E+00	0.000E+00	0.000E+00
4-Me-c-2-Pentene	0.000E+00	0.000E+00	0.000E+00
2-methyl-1-pentene	0.000E+00	0.000E+00	0.000E+00
c-3-hexene	3.149E-01	3.149E-01	3.149E-01
3-MeCyclopentene	0.000E+00	0.000E+00	0.000E+00
1-methylcyclopentene	6.002E-01	6.002E-01	6.002E-01
3-Me-1-Hexene	7.085E-02	7.085E-02	7.085E-02
2-Methyl-2-hexene	0.000E+00	0.000E+00	0.000E+00
3-ethyl-c-2-pentene	3.240E-02	3.240E-02	3.240E-02
2,3-DMe-2-Pentene	7.800E-02	7.800E-02	7.800E-02
2,4,4-Trimethyl-2-Pentene	2.044E-02	2.044E-02	2.044E-02
1-MethylCycloHexene	0.000E+00	0.000E+00	0.000E+00
1-Undecene	2.527E-04	2.527E-04	2.527E-04
1-Dodecene	4.272E-04	4.272E-04	4.272E-04
OXYGENATE			
MTBE	9.119E+00	9.119E+00	9.119E+00
ETBE	0.000E+00	0.000E+00	0.000E+00
OTHER			
Ethyne	0.000E+00	0.000E+00	0.000E+00
Propyne	0.000E+00	0.000E+00	0.000E+00
Propadiene	0.000E+00	0.000E+00	0.000E+00
Indan	6.600E-03	6.600E-03	6.600E-03
Cyclohexene	0.000E+00	0.000E+00	0.000E+00
	9.586E+01	9.586E+01	9.586E+01

Compound Data Sheet **p. 1 of 4**

Compounds	Formula	Tb(C)	Tb (K)	MW
PARAFFINS				
Methane	CH4	-161.45	111.55	16
Ethane	C2H6	-88.6	184.40	30.1
Propane	C3H8	-42.1	230.90	44.1
Butane	C4H10	-0.5	272.50	58.12
n-Pentane	C5H12	36.07	309.07	72.15
n-Hexane	C6H14	68.73	341.73	86.18
n-Heptane	C7H16	98.43	371.43	100.75
n-Octane	C8H18	125.67	398.67	114.22
n-Nonane	C9H20	150.80	423.80	128.25
n-Decane	C10H22	174.12	447.12	142.28
n-Undecane	C11H24	195.90	468.90	156.3
n-Dodecane	C12H26	216.28	489.28	170.34
n-Tridecane	C13H28	235.40	508.40	184.37
n-Tetradecane	C14H30	253.70	526.70	198.4
n-Pentadecane	C15H32	268.17	541.17	212.42
ISOPARAFFINS				
Isobutane	C4H10	-11.7	261.30	58.1
2,2-dimethylpropane	C5H12	10	283.00	72.15
Isopentane	C5H12	27.83	300.83	72.15
2,3-Dimethylbutane	C5H12	57.98	330.98	86.18
2-Methylpentane	C6H14	60.26	333.26	86.18
3-Methylpentane	C6H14	63.27	336.27	86.18
2,2-Dimethylpentane	C7H16	79.19	352.19	100.75
2,4-Dimethylpentane	C7H16	80.49	353.49	100.75
2,2,3-Trimethylbutane	C7H16	80.88	353.88	100.75
3,3-Dimethylpentane	C7H16	86.06	359.06	100.75
2-Methylhexane	C7H16	90.05	363.05	100.75
2,3-Dimethylpentane	C7H16	91.31	364.31	100.75
3-Methylhexane	C7H16	91.84	364.84	100.75
3-Ethylpentane	C7H16	93.47	366.47	100.75
2,2-Dimethylhexane	C8H18	106.84	379.84	114.22
2,5-Dimethylhexane	C8H18	109.11	382.11	114.22
2,2,3-Trimethylpentane	C8H18	109.84	382.84	114.22
2,4-Dimethylhexane	C8H18	109.43	382.43	114.22
2,3-Dimethylhexane	C8H18	115.61	388.61	114.22
2-Methylheptane	C8H18	117.31	390.31	114.22
4-Methylheptane	C8H18	117.71	390.71	114.22
3-Methylheptane	C8H18	118.00	391.00	114.22
3-Ethylhexane	C8H18	118.53	391.53	114.22
2,5-Dimethylheptane	C8H18	136.00	409.00	128.25
3,5-Dimethylheptane (D)	C8H18	136.00	409.00	128.25
3,3-Dimethylheptane	C8H18	137.01	410.01	128.25
3,5-Dimethylheptane (L)	C8H18	136.00	409.00	128.25
2,3-Dimethylheptane	C8H18	140.50	413.50	128.25
3,4-Dimethylheptane (D)	C8H18	140.61	413.61	128.25
3,4-Dimethylheptane (L)	C8H18	140.61	413.61	128.25
2-Methyloctane	C9H20	143.26	416.26	128.25
3-Methyloctane	C9H20	143.50	416.50	128.25

3,3-Diethylpentane	C9H20	147.17	420.17	128.25
2,2-Dimethyloctane	C10H22	156.89	429.89	142.28
3,3-Dimethyloctane	C10H22	161.22	434.22	142.28
2,3-Dimethyloctane	C10H22	164.31	437.31	142.28
2-Methylnonane	C10H22	167.00	440.00	142.28
3-Ethyloctane	C10H22	167.78	440.78	142.28
3-Methylnonane	C10H22	168.00	441.00	142.28
2,2-dimethylbutane	C6H14	49.7	322.70	86.177
2,2,4-TriMePentane	C8H18	99.2	372.20	114.23
3,3-Dimethylhexane	C8H18	112	385.00	114.23
2,3,4-Trimethylpentane	C8H18	113	386.00	114.23
2,3-MethylEthylPentane	C8H18	116	389.00	114.23
2,3,5-trimethylhexane	C9H20	131	404.00	128.26
2,4-Dimethylheptane	C9H20	133	406.00	128.26
4-Methyloctane	C9H20	142	415.00	128.26
AROMATICS				
Benzene	C6H6	80.09	353.09	78.11
Toluene	C7H8	110.62	383.62	92.13
Ethylbenzene	C8H10	136.19	409.19	106.16
m-Xylene	C8H10	139.10	412.10	106.16
p-Xylene	C8H10	138.35	411.35	106.16
o-Xylene	C8H10	144.42	417.42	106.16
Isopropylbenzene	CCH5CH(CH3)2	152.39	425.39	120.19
n-Propylbenzene	C9H12	159.22	432.22	120.19
1-Methyl-3-Ethylbenzene	C9H12	161.30	434.30	120.19
1-Methyl-4-Ethylbenzene	C9H12	161.98	434.98	120.19
1,3,5-Trimethylbenzene	C9H12	164.71	437.71	120.19
1-Methyl-2-Ethylbenzene	C9H12	165.15	438.15	120.19
1,2,4-Trimethylbenzene	C9H12	169.34	442.34	120.19
tert-Butylbenzene	C10H14	169.11	442.11	134.12
Isobutylbenzene	C10H14	172.76	445.76	134.12
sec-Butylbenzene	C10H14	173.30	446.30	134.12
1-Methyl-3-Isopropylbenzene	C10H14	175.78	448.78	134.12
1-Methyl-4-Isopropylbenzene	C10H14	177.10	450.10	134.12
1-Methyl-2-Isopropylbenzene	C10H14	178.15	451.15	134.12
1-Methyl-3-n-Propylbenzene	C10H14	182.01	455.01	134.12
1-Methyl-4-n-Propylbenzene	C10H14	183.42	456.42	134.12
n-Butylbenzene	C10H14	183.27	456.27	134.12
1,3-Dimethyl-5-Ethylbenzene	C10H14	183.76	456.76	134.12
1,2-Diethylbenzene	C10H14	183.42	456.42	134.12
1-Methyl-2-n-Propylbenzene	C10H14	184.97	457.97	134.12
1,4-Dimethyl-2-Ethylbenzene	C10H14	186.83	459.83	134.12
1,2-Dimethyl-4-Ethylbenzene	C10H14	189.48	462.48	134.12
1,3-Dimethyl-2-Ethylbenzene	C10H14	190.01	463.01	134.12
1,2-Dimethyl-3-Ethylbenzene	C10H14	193.91	466.91	134.12
1,2,4,5-Tetramethylbenzene	C10H14	196.80	469.80	134.12
2-Methylbutylbenzene	C10H14	196.67	469.67	148.24
tert-1-Butyl-2-Methylbenzene	C10H14	198.89	471.89	148.24
n-Pentylbenzene	C11H16	205.40	478.40	148.24
t-1-Butyl-3,5-Dimethylbenzene	C12H18	204.44	477.44	162.26
t-1-Butyl-4-Ethylbenzene	C12H18	206.11	479.11	162.26
1,3,5-Triethylbenzene	C12H18	216.00	489.00	162.26
1,2,4-Triethylbenzene	C12H18	217.70	490.70	162.26

n-Hexylbenzene	C12H18	226.11	499.11	162.26
1,2,3-TrimethylBenzene	C9H12	175	448.00	120.19
1,3-Diethylbenzene	C10H14	181	454.00	134.22
1,4-Diethylbenzene	C10H14	184	457.00	134.22
1,2,3,5-Tetramethylbenzene	C10H14	197.9	470.90	134.22
1,2,3,4-Tetramethylbenzene	C10H14	205	478.00	134.22
Amylbenzene	C11H16	205	478.00	148.25
1,4-Diisopropylbenzene	C12H18	203	476.00	162.27
Naphthalene	C10H8	218	491.00	128.17
NAPTHENES				
Cyclopentane	C5H10	49.26	322.26	70.13
Methylcyclopentane	C6H12	71.81	344.81	84.16
Cyclohexane	C6H12	80.72	353.72	84.16
1,1-Dimethylcyclopentane	C7H14	87.84	360.84	98.18
cis-1,3-Dimethylcyclopentane	C7H14	90.77	363.77	98.18
trans-1,3-Dimethylcyclopentane	C7H14	91.72	364.72	98.18
trans-1,2-Dimethylcyclopentane	C7H14	91.87	364.87	98.18
Methylcyclohexane	C7H14	96.01	369.01	98.18
Ethylcyclopentane	C7H14	103.47	376.47	98.18
ctc-1,2,4-Trimethylcyclopentane	C8H16	109.29	382.29	112.21
ctc-1,2,3-Trimethylcyclopentane	C8H16	110.22	383.22	112.21
cct-1,2,4-Trimethylcyclopentane	C8H16	116.73	389.73	112.21
trans-1,4-Dimethylcyclohexane	C8H16	119.41	392.41	112.21
1-Ethyl-1-Methylcyclopentane	C8H16	121.52	394.52	112.21
trans-1,2-Dimethylcyclohexane	C8H16	123.42	396.42	112.21
ccc-1,2,3-Trimethylcyclopentane	C8H16	123.00	396.00	112.21
Isopropylcyclopentane	C8H16	126.40	399.40	112.21
cis-1,2-Dimethylcyclohexane	C8H16	129.73	402.73	112.21
n-Propylcyclopentane	C8H16	130.95	403.95	112.21
ccc-1,3,5-Trimethylcyclohexane	C9H18	138.41	411.41	126.23
1,1,4-Trimethylcyclohexane	C9H18	135.00	408.00	126.23
ctt-1,2,4-Trimethylcyclohexane	C9H18	141.24	414.24	126.23
ctc-1,2,4-Trimethylcyclohexane	C9H18	147.78	420.78	126.23
1,1,2-Trimethylcyclohexane	C9H18	146.00	419.00	126.23
Isobutylcyclopentane	C9H18	148.00	421.00	126.23
Isopropylcyclohexane	C9H18	154.57	427.57	126.23
n-Butylcyclopentane	C9H18	156.56	429.56	126.23
Isobutylcyclohexane	C10H20	171.29	444.29	140.26
t-1-Methyl-2-Propylcyclohexane	C10H20	176.67	449.67	140.26
t-1-Methyl-2-(4MP)cyclopentane	C12H24	204.44	477.44	168.33
cis-1,3-Dimethylcyclohexane	C8H16	120	393.00	112.21
2,2,5-Trimethylhexane	C9H20	124	397.00	128.26
1,1-Dimethylcyclohexane	C8H16	120	393.00	112.21
Ethylcyclohexane	C8H16	132	405.00	112.21
c-1,4-Dimethylcyclohexane	C8H16	120	393.00	112.21
OLEFINS				
Isobutene	C4H8	-6.89	266.11	56.11
1-Butene	C4H8	-6.25	266.75	56.11
cis-2-Butene	C4H8	3.72	276.72	56.11
3-Methyl-1-Butene	C5H10	20.06	293.06	70.13
1-Pentene	C5H10	29.97	302.97	70.13
2-Methyl-1-Butene	C5H10	31.16	304.16	70.13
2-Methyl-1,3-Butadiene	C5H8	34.00	307.00	70.13
trans-2-Pentene	C5H10	36.36	309.36	70.13

cis-2-Pentene	C5H10	36.94	309.94	70.13
4-Methylpentene-1	C6H12	53.87	326.87	84.16
1-Hexene	C6H12	63.48	336.48	84.16
trans-2-Hexene	C6H12	67.88	340.88	84.16
2-Methylpentene-2	C6H12	67.31	340.31	84.16
cis-2-Hexene	C6H12	68.88	341.88	84.16
1-Heptene	C7H14	93.64	366.64	98.19
trans-3-Heptene	C7H14	95.67	368.67	98.19
cis-3-Heptene	C7H14	95.75	368.75	98.19
trans-2-Heptene	C7H14	97.95	370.95	98.19
cis-2-Heptene	C7H14	98.41	371.41	98.19
1-Octene	C8H16	121.27	394.27	112.22
trans-2-Octene	C8H16	125.00	398.00	112.22
cis-2-Octene	C8H16	125.61	398.61	112.22
1-Nonene	C9H18	146.89	419.89	126.24
trans-3-Nonene	C9H18	147.70	420.70	126.24
cis-3-Nonene	C9H18	147.70	420.70	126.24
trans-2-Nonene	C9H18	148.50	421.50	126.24
cis-2-Nonene	C9H18	148.50	421.50	126.24
1-Decene	C10H20	170.60	443.60	140.25
2-methylpropene	C4H8	-6.9	266.10	56.107
t-2-butene	C4H8	**3.72**	276.72	56.107
2-methyl-2-butene	C5H10	39	312.00	70.134
cyclopentadiene	C5H6	42	315.00	66.102
cyclopentene	C5H8	44	317.00	68.118
3-methyl-1-pentene	C6H12	54	327.00	84.161
4-Me-c-2-Pentene	C6H12	57.5	330.50	84.161
2-methyl-1-pentene	C6H12	62	335.00	84.161
c-3-hexene	C6H12	67	340.00	84.161
3-MeCyclopentene	C6H10	65	338.00	82.145
1-methylcyclopentene	C6H10	72	345.00	82.145
3-Me-1-Hexene	C7H14	84	357.00	98.188
2-Methyl-2-hexene	C7H14	95	368.00	98.188
3-ethyl-c-2-pentene	C7H14	96	369.00	98.188
2,3-DMe-2-Pentene	C7H14	97	370.00	98.188
2,4,4-Trimethyl-2-Pentene	C8H16	105	378.00	112.21
1-MethylCycloHexene	C7H12	110	383.00	96.172
1-Undecene	C11H22	193	466.00	154.29
1-Dodecene	C12H24	213	486.00	168.32
OXYGENATE				
MTBE	C5H12O	55.20	328.20	88.2
ETBE	C6H14O	70.00	343.00	102.2
OTHER				
Ethyne	C2H2	-28.10	244.90	26
Propyne	C3H4	-23.00	250.00	40.1
Propadiene	C3H4	-34.50	238.50	40.1
Indan	C9H10	176.5	449.50	118.18
Cyclohexene	C6H10	83	356.00	82.145

1. Compound vapor pressure calculated using V.P.(atm) = exp{19*(1-(Tbi/T)+8.5(ln(Tbi/T)))
Tbi = compound boiling point (degree K), T = temperature (degree K)

Hot Soak Speciated Emissions

RVP (psia)	Temp (F)	Temp (R)	Temp (K)	Gasoline V.P. (psia)	Liquid MW	Vapor MW	Vapor Mr
7	105	564.6	313.56	8.10	91.85	68.00	0.049

Regular Emitter (vapor)

Compound	Liquid comp. (% by mass)	MW	Boiling pt. (deg C)	Boiling pt. (deg K)	Compound V.P. (psia)	Liquid Mole Fraction	Compound Pp (psia)	Compound Mr	Vapor Mole Fraction	Compound Specific Adj. Factor	Vapor-based speciated emissions (% by mass)
PARAFFINS											
Methane	0	16	-161.45	111.55	4.66E+02	0.00E+00	0.00E+00	0.097	0.00E+00	1	0.000E+00
Ethane	0	30.1	-88.60	184.40	4.04E+02	0.00E+00	0.00E+00	0.068	0.00E+00	1	0.000E+00
Propane	0	44.1	-42.10	230.90	1.63E+02	0.00E+00	0.00E+00	0.057	0.00E+00	1	0.000E+00
Butane	0.22	58.12	-0.50	272.50	5.37E+01	3.48E-03	1.87E-01	0.052	2.36E-02	1	2.018E+00
n-Pentane	4.01	72.15	36.07	309.07	1.71E+01	5.11E-02	8.71E-01	0.048	1.07E-01	1	1.132E+01
n-Hexane	1.8	86.18	68.73	341.73	5.54E+00	1.92E-02	1.06E-01	0.046	1.27E-02	1	1.610E+00
n-Heptane	1.21	100.75	98.43	371.43	1.86E+00	1.10E-02	2.05E-02	0.044	2.41E-03	1	3.567E-01
n-Octane	0.73	114.22	125.67	398.67	6.52E-01	5.87E-03	3.83E-03	0.043	4.43E-04	1	7.439E-02
n-Nonane	0.22	128.25	150.80	423.80	2.39E-01	1.58E-03	3.76E-04	0.042	4.31E-05	1	8.128E-03
n-Decane	0.14	142.28	174.12	447.12	9.17E-02	9.04E-04	8.29E-05	0.042	9.40E-06	1	1.967E-03
n-Undecane	0.12	156.3	195.90	468.90	3.67E-02	7.05E-04	2.59E-05	0.041	2.91E-06	1	6.698E-04
n-Dodecane	0.09	170.34	216.28	489.28	1.53E-02	4.85E-04	7.44E-06	0.040	8.32E-07	1	2.084E-04
n-Tridecane	0	184.37	235.40	508.40	6.67E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Tetradecane	0	198.4	253.70	526.70	2.97E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Pentadecane	0	212.42	268.17	541.17	1.56E-03	0.00E+00	0.00E+00	0.039	0.00E+00	1	0.000E+00
ISOPARAFFINS										1	
Isobutane	0.05	58.1	-11.70	261.30	7.40E+01	7.90E-04	5.85E-02	0.052	7.41E-03	1	6.330E-01
2,2-dimethylpropane	0	72.15	10.00	283.00	3.92E+01	0.00E+00	0.00E+00	0.048	0.00E+00	1	0.000E+00
Isopentane	8.89	72.15	27.83	300.83	2.23E+01	1.13E-01	2.53E+00	0.048	3.10E-01	1	3.285E+01
2,3-Dimethylbutane	1.98	86.18	57.98	330.98	8.10E+00	2.11E-02	1.71E-01	0.046	2.04E-02	1	2.589E+00
2-Methylpentane	3.97	86.18	60.26	333.26	7.48E+00	4.23E-02	3.16E-01	0.046	3.78E-02	1	4.792E+00
3-Methylpentane	2.19	86.18	63.27	336.27	6.73E+00	2.33E-02	1.57E-01	0.046	1.88E-02	1	2.378E+00
2,2-Dimethylpentane	0.08	100.75	79.19	352.19	3.80E+00	7.29E-04	2.77E-03	0.044	3.25E-04	1	4.815E-02
2,4-Dimethylpentane	0.41	100.75	80.49	353.49	3.62E+00	3.74E-03	1.35E-02	0.044	1.59E-03	1	2.353E-01
2,2,3-Trimethylbutane	0.03	100.75	80.88	353.88	3.57E+00	2.74E-04	9.77E-04	0.044	1.15E-04	1	1.698E-02
3,3-Dimethylpentane	0.08	100.75	86.06	359.06	2.95E+00	7.29E-04	2.15E-03	0.044	2.53E-04	1	3.742E-02
2-Methylhexane	1.59	100.75	90.05	363.05	2.55E+00	1.45E-02	3.69E-02	0.044	4.33E-03	1	6.415E-01
2,3-Dimethylpentane	0.27	100.75	91.31	364.31	2.43E+00	2.46E-03	5.98E-03	0.044	7.02E-04	1	1.039E-01
3-Methylhexane	1.4	100.75	91.84	364.84	2.38E+00	1.28E-02	3.04E-02	0.044	3.57E-03	1	5.283E-01
3-Ethylpentane	0	100.75	93.47	366.47	2.24E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
2,2-Dimethylhexane	0.27	114.22	106.84	379.84	1.35E+00	2.17E-03	2.94E-03	0.043	3.40E-04	1	5.707E-02
2,5-Dimethylhexane	0.16	114.22	109.11	382.11	1.24E+00	1.29E-03	1.59E-03	0.043	1.85E-04	1	3.101E-02
2,2,3-Trimethylpentane	0	114.22	109.84	382.84	1.21E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,4-Dimethylhexane	0.51	114.22	109.43	382.43	1.22E+00	4.10E-03	5.02E-03	0.043	5.81E-04	1	9.763E-02
2,3-Dimethylhexane	0.29	114.22	115.61	388.61	9.65E-01	2.33E-03	2.25E-03	0.043	2.60E-04	1	4.375E-02
2-Methylheptane	0.65	114.22	117.31	390.31	9.03E-01	5.23E-03	4.72E-03	0.043	5.46E-04	1	9.179E-02
4-Methylheptane	0.37	114.22	117.71	390.71	8.89E-01	2.98E-03	2.65E-03	0.043	3.06E-04	1	5.144E-02
3-Methylheptane	0.87	114.22	118.00	391.00	8.79E-01	7.00E-03	6.15E-03	0.043	7.12E-04	1	1.196E-01
3-Ethylhexane	0	114.22	118.53	391.53	8.61E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,5-Dimethylheptane	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (D)	0.37	128.25	136.00	409.00	4.33E-01	2.65E-03	1.15E-03	0.042	1.31E-04	1	2.478E-02
3,3-Dimethylheptane	0	128.25	137.01	410.01	4.16E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (L)	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethylheptane	0.05	128.25	140.50	413.50	3.62E-01	3.58E-04	1.30E-04	0.042	1.48E-05	1	2.798E-03

3,4-Dimethylheptane (D)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,4-Dimethylheptane (L)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methyloctane	0	128.25	143.26	416.26	3.24E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methyloctane	0.38	128.25	143.50	416.50	3.21E-01	2.72E-03	8.73E-04	0.042	1.00E-04	1	1.885E-02
3,3-Diethylpentane	0	128.25	147.17	420.17	2.77E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-Dimethyloctane	0.06	142.28	156.89	429.89	1.87E-01	3.87E-04	7.22E-05	0.042	8.19E-06	1	1.715E-03
3,3-Dimethyloctane	0	142.28	161.22	434.22	1.56E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethyloctane	0	142.28	164.31	437.31	1.38E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methylnonane	0	142.28	167.00	440.00	1.23E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Ethyloctane	0	142.28	167.78	440.78	1.19E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methylnonane	0	142.28	168.00	441.00	1.18E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-dimethylbutane	0.44	86.177	49.70	322.70	1.08E+01	4.69E-03	5.06E-02	0.046	6.04E-03	1	7.660E-01
2,2,4-TriMePentane	0.61	114.23	99.20	372.20	1.81E+00	4.91E-03	8.86E-03	0.043	1.03E-03	1	1.724E-01
3,3-Dimethylhexane	0.19	114.23	112.00	385.00	1.11E+00	1.53E-03	1.69E-03	0.043	1.96E-04	1	3.295E-02
2,3,4-Trimethylpentane	0.48	114.23	113.00	386.00	1.07E+00	3.86E-03	4.12E-03	0.043	4.77E-04	1	8.009E-02
2,3-MethylEthylPentane	0	114.23	116.00	389.00	9.50E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,3,5-trimethylhexane	0.05	128.26	131.00	404.00	5.28E-01	3.58E-04	1.89E-04	0.042	2.16E-05	1	4.083E-03
2,4-Dimethylheptane	0.17	128.26	133.00	406.00	4.88E-01	1.22E-03	5.94E-04	0.042	6.80E-05	1	1.283E-02
4-Methyloctane	0.48	128.26	142.00	415.00	3.41E-01	3.44E-03	1.17E-03	0.042	1.34E-04	1	2.529E-02
AROMATICS										1	
Benzene	1.42	78.11	80.09	353.09	3.67E+00	1.67E-02	6.14E-02	0.047	7.43E-03	1	8.532E-01
Toluene	7.17	92.13	110.62	383.62	1.17E+00	7.15E-02	8.36E-02	0.045	9.91E-03	1	1.342E+00
Ethylbenzene	1.04	106.16	136.19	409.19	4.30E-01	9.00E-03	3.87E-03	0.044	4.51E-04	1	7.043E-02
m-Xylene	3.34	106.16	139.10	412.10	3.83E-01	2.89E-02	1.11E-02	0.044	1.29E-03	1	2.014E-01
p-Xylene	0	106.16	138.35	411.35	3.94E-01	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
o-Xylene	1.41	106.16	144.42	417.42	3.09E-01	1.22E-02	3.77E-03	0.044	4.40E-04	1	6.870E-02
Isopropylbenzene	0.1	120.19	152.39	425.39	2.24E-01	7.64E-04	1.71E-04	0.043	1.97E-05	1	3.485E-03
n-Propylbenzene	0.52	120.19	159.22	432.22	1.70E-01	3.97E-03	6.74E-04	0.043	7.76E-05	1	1.372E-02
1-Methyl-3-Ethylbenzene	1.81	120.19	161.30	434.30	1.56E-01	1.38E-02	2.15E-03	0.043	2.48E-04	1	4.385E-02
1-Methyl-4-Ethylbenzene	0.81	120.19	161.98	434.98	1.51E-01	6.19E-03	9.37E-04	0.043	1.08E-04	1	1.908E-02
1,3,5-Trimethylbenzene	0.94	120.19	164.71	437.71	1.35E-01	7.18E-03	9.72E-04	0.043	1.12E-04	1	1.979E-02
1-Methyl-2-Ethylbenzene	0	120.19	165.15	438.15	1.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
1,2,4-Trimethylbenzene	2.72	120.19	169.34	442.34	1.12E-01	2.08E-02	2.32E-03	0.043	2.68E-04	1	4.730E-02
tert-Butylbenzene	0	134.12	169.11	442.11	1.13E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylbenzene	0.06	134.12	172.76	445.76	9.70E-02	4.11E-04	3.99E-05	0.042	4.55E-06	1	8.967E-04
sec-Butylbenzene	0.06	134.12	173.30	446.30	9.49E-02	4.11E-04	3.90E-05	0.042	4.44E-06	1	8.766E-04
1-Methyl-3-Isopropylbenzene	0	134.12	175.78	448.78	8.56E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-4-Isopropylbenzene	0.07	134.12	177.10	450.10	8.10E-02	4.79E-04	3.88E-05	0.042	4.43E-06	1	8.731E-04
1-Methyl-2-Isopropylbenzene	0	134.12	178.15	451.15	7.75E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-3-n-Propylbenzene	0.44	134.12	182.01	455.01	6.60E-02	3.01E-03	1.99E-04	0.042	2.27E-05	1	4.469E-03
1-Methyl-4-n-Propylbenzene	0.04	134.12	183.42	456.42	6.22E-02	2.74E-04	1.70E-05	0.042	1.94E-06	1	3.830E-04
n-Butylbenzene	0.07	134.12	183.27	456.27	6.26E-02	4.79E-04	3.00E-05	0.042	3.42E-06	1	6.744E-04
1,3-Dimethyl-5-Ethylbenzene	0	134.12	183.76	456.76	6.13E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2-Diethylbenzene	0.06	134.12	183.42	456.42	6.22E-02	4.11E-04	2.55E-05	0.042	2.91E-06	1	5.744E-04
1-Methyl-2-n-Propylbenzene	0.21	134.12	184.97	457.97	5.82E-02	1.44E-03	8.38E-05	0.042	9.55E-06	1	1.884E-03
1,4-Dimethyl-2-Ethylbenzene	0.39	134.12	186.83	459.83	5.39E-02	2.67E-03	1.44E-04	0.042	1.64E-05	1	3.236E-03
1,2-Dimethyl-4-Ethylbenzene	0.48	134.12	189.48	462.48	4.82E-02	3.29E-03	1.58E-04	0.042	1.81E-05	1	3.561E-03
1,3-Dimethyl-2-Ethylbenzene	0.25	134.12	190.01	463.01	4.71E-02	1.71E-03	8.06E-05	0.042	9.19E-06	1	1.814E-03
1,2-Dimethyl-3-Ethylbenzene	0	134.12	193.91	466.91	3.99E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2,4,5-Tetramethylbenzene	0.26	134.12	196.80	469.80	3.53E-02	1.78E-03	6.29E-05	0.042	7.17E-06	1	1.415E-03

2-Methylbutylbenzene	0	148.24	196.67	469.67	3.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
tert-1-Butyl-2-Methylbenzene	0	148.24	198.89	471.89	3.23E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Pentylbenzene	0	148.24	205.40	478.40	2.45E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-3,5-Dimethylbenzene	0	162.26	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-4-Ethylbenzene	0	162.26	206.11	479.11	2.37E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,3,5-Triethylbenzene	0	162.26	216.00	489.00	1.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,4-Triethylbenzene	0	162.26	217.70	490.70	1.44E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Hexylbenzene	0	162.26	226.11	499.11	1.00E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,3-TrimethylBenzene	0.67	120.19	175.00	448.00	8.84E-02	5.12E-03	4.53E-04	0.043	5.21E-05	1	9.214E-03
1,3-Diethylbenzene	0.22	134.22	181.00	454.00	6.88E-02	1.51E-03	1.04E-04	0.042	1.18E-05	1	2.331E-03
1,4-Diethylbenzene	0.85	134.22	184.00	457.00	6.07E-02	5.82E-03	3.53E-04	0.042	4.02E-05	1	7.942E-03
1,2,3,5-Tetramethylbenzene	0.39	134.22	197.90	470.90	3.37E-02	2.67E-03	9.00E-05	0.042	1.03E-05	1	2.025E-03
1,2,3,4-Tetramethylbenzene	0.18	134.22	205.00	478.00	2.49E-02	1.23E-03	3.07E-05	0.042	3.50E-06	1	6.902E-04
Amylbenzene	0	148.25	205.00	478.00	2.49E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,4-Diisopropylbenzene	0.01	162.27	203.00	476.00	2.71E-02	5.66E-05	1.54E-06	0.041	1.72E-07	1	4.113E-05
Naphthalene	0.39	128.17	218.00	491.00	1.42E-02	2.79E-03	3.98E-05	0.042	4.55E-06	1	8.581E-04
NAPTHENES										1	
Cyclopentane	0	70.13	49.26	322.26	1.09E+01	0.00E+00	0.00E+00	0.049	0.00E+00	1	0.000E+00
Methylcyclopentane	1.68	84.16	71.81	344.81	4.96E+00	1.83E-02	9.10E-02	0.046	1.09E-02	1	1.350E+00
Cyclohexane	0.52	84.16	80.72	353.72	3.59E+00	5.68E-03	2.04E-02	0.046	2.44E-03	1	3.024E-01
1,1-Dimethylcyclopentane	0	98.18	87.84	360.84	2.76E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclopentane	0.42	98.18	90.77	363.77	2.48E+00	3.93E-03	9.74E-03	0.045	1.15E-03	1	1.654E-01
trans-1,3-Dimethylcyclopentane	0	98.18	91.72	364.72	2.39E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclopentane	0.71	98.18	91.87	364.87	2.38E+00	6.64E-03	1.58E-02	0.045	1.86E-03	1	2.685E-01
Methylcyclohexane	0.84	98.18	96.01	369.01	2.04E+00	7.86E-03	1.60E-02	0.045	1.88E-03	1	2.720E-01
Ethylcyclopentane	0	98.18	103.47	376.47	1.54E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclopentane	0	112.21	109.29	382.29	1.23E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ctc-1,2,3-Trimethylcyclopentane	0	112.21	110.22	383.22	1.19E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cct-1,2,4-Trimethylcyclopentane	0	112.21	116.73	389.73	9.24E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,4-Dimethylcyclohexane	0.07	112.21	119.41	392.41	8.32E-01	5.73E-04	4.77E-04	0.043	5.53E-05	1	9.128E-03
1-Ethyl-1-Methylcyclopentane	0	112.21	121.52	394.52	7.67E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclohexane	0.17	112.21	123.42	396.42	7.12E-01	1.39E-03	9.90E-04	0.043	1.15E-04	1	1.896E-02
ccc-1,2,3-Trimethylcyclopentane	0	112.21	123.00	396.00	7.23E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
Isopropylcyclopentane	0	112.21	126.40	399.40	6.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-1,2-Dimethylcyclohexane	0.06	112.21	129.73	402.73	5.55E-01	4.91E-04	2.73E-04	0.043	3.16E-05	1	5.220E-03
n-Propylcyclopentane	0	112.21	130.95	403.95	5.29E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ccc-1,3,5-Trimethylcyclohexane	0	126.23	138.41	411.41	3.93E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,4-Trimethylcyclohexane	0	126.23	135.00	408.00	4.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctt-1,2,4-Trimethylcyclohexane	0	126.23	141.24	414.24	3.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclohexane	0	126.23	147.78	420.78	2.70E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,2-Trimethylcyclohexane	0	126.23	146.00	419.00	2.90E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclopentane	0	126.23	148.00	421.00	2.68E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isopropylcyclohexane	0	126.23	154.57	427.57	2.05E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
n-Butylcyclopentane	0	126.23	156.56	429.56	1.89E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclohexane	0	140.26	171.29	444.29	1.03E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-Propylcyclohexane	0	140.26	176.67	449.67	8.25E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-(4MP)cyclopentane	0	168.33	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclohexane	0.26	112.21	120.00	393.00	8.13E-01	2.13E-03	1.73E-03	0.043	2.01E-04	1	3.313E-02
2,2,5-Trimethylhexane	0.15	128.26	124.00	397.00	6.96E-01	1.07E-03	7.47E-04	0.042	8.55E-05	1	1.614E-02
1,1-Dimethylcyclohexane	0.25	112.21	120.00	393.00	8.13E-01	2.05E-03	1.66E-03	0.043	1.93E-04	1	3.186E-02
Ethylcyclohexane	0.07	112.21	132.00	405.00	5.08E-01	5.73E-04	2.91E-04	0.043	3.37E-05	1	5.566E-03
c-1,4-Dimethylcyclohexane	0.29	112.21	120.00	393.00	8.13E-01	2.37E-03	1.93E-03	0.043	2.24E-04	1	3.695E-02
OLEFINS										1	
Isobutene	0.04	56.11	-6.89	266.11	6.46E+01	6.55E-04	4.23E-02	0.052	5.39E-03	1	4.445E-01
1-Butene	0	56.11	-6.25	266.75	6.34E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
cis-2-Butene	0.14	56.11	3.72	276.72	4.74E+01	2.29E-03	1.09E-01	0.052	1.38E-02	1	1.140E+00

3-Methyl-1-Butene	0.08	70.13	20.06	293.06	2.87E+01	1.05E-03	3.00E-02	0.049	3.69E-03	1	3.805E-01
1-Pentene	0.25	70.13	29.97	302.97	2.09E+01	3.27E-03	6.83E-02	0.049	8.39E-03	1	8.655E-01
2-Methyl-1-Butene	0.22	70.13	31.16	304.16	2.01E+01	2.88E-03	5.78E-02	0.049	7.10E-03	1	7.325E-01
2-Methyl-1,3-Butadiene	0.02	70.13	34.00	307.00	1.83E+01	2.62E-04	4.79E-03	0.049	5.88E-04	1	6.068E-02
trans-2-Pentene	1.62	70.13	36.36	309.36	1.69E+01	2.12E-02	3.59E-01	0.049	4.41E-02	1	4.547E+00
cis-2-Pentene	0.75	70.13	36.94	309.94	1.66E+01	9.82E-03	1.63E-01	0.049	2.00E-02	1	2.064E+00
4-Methylpentene-1	0.25	84.16	53.87	326.87	9.34E+00	2.73E-03	2.55E-02	0.046	3.06E-03	1	3.782E-01
1-Hexene	0.77	84.16	63.48	336.48	6.68E+00	8.40E-03	5.61E-02	0.046	6.72E-03	1	8.323E-01
trans-2-Hexene	0.85	84.16	67.88	340.88	5.71E+00	9.28E-03	5.30E-02	0.046	6.35E-03	1	7.859E-01
2-Methylpentene-2	0.66	84.16	67.31	340.31	5.83E+00	7.20E-03	4.20E-02	0.046	5.03E-03	1	6.229E-01
cis-2-Hexene	0.54	84.16	68.88	341.88	5.51E+00	5.89E-03	3.25E-02	0.046	3.89E-03	1	4.817E-01
1-Heptene	0.12	98.19	93.64	366.64	2.23E+00	1.12E-03	2.50E-03	0.045	2.94E-04	1	4.247E-02
trans-3-Heptene	0.32	98.19	95.67	368.67	2.06E+00	2.99E-03	6.18E-03	0.045	7.27E-04	1	1.049E-01
cis-3-Heptene	0.88	98.19	95.75	368.75	2.06E+00	8.23E-03	1.69E-02	0.045	1.99E-03	1	2.878E-01
trans-2-Heptene	0.28	98.19	97.95	370.95	1.89E+00	2.62E-03	4.96E-03	0.045	5.84E-04	1	8.429E-02
cis-2-Heptene	0.43	98.19	98.41	371.41	1.86E+00	4.02E-03	7.49E-03	0.045	8.81E-04	1	1.272E-01
1-Octene	0	112.22	121.27	394.27	7.74E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-2-Octene	0	112.22	125.00	398.00	6.69E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-2-Octene	0.06	112.22	125.61	398.61	6.53E-01	4.91E-04	3.21E-04	0.043	3.72E-05	1	6.138E-03
1-Nonene	0.2	126.24	146.89	419.89	2.80E-01	1.46E-03	4.07E-04	0.042	4.67E-05	1	8.669E-03
trans-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
trans-2-Nonene	0	126.24	148.50	421.50	2.62E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-2-Nonene	0.06	126.24	148.50	421.50	2.62E-01	4.37E-04	1.14E-04	0.042	1.31E-05	1	2.437E-03
1-Decene	0	140.25	170.60	443.60	1.06E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-methylpropene	0	56.107	-6.90	266.10	6.46E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
t-2-butene	0.19	56.107	3.72	276.72	4.74E+01	3.11E-03	1.47E-01	0.052	1.88E-02	1	1.547E+00
2-methyl-2-butene	0.86	70.134	39.00	312.00	1.55E+01	1.13E-02	1.74E-01	0.049	2.14E-02	1	2.211E+00
cyclopentadiene	0.02	66.102	42.00	315.00	1.40E+01	2.78E-04	3.89E-03	0.050	4.83E-04	1	4.691E-02
cyclopentene	0.32	68.118	44.00	317.00	1.31E+01	4.31E-03	5.65E-02	0.049	6.97E-03	1	6.985E-01
3-methyl-1-pentene	0	84.161	54.00	327.00	9.30E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
4-Me-c-2-Pentene	0	84.161	57.50	330.50	8.24E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
2-methyl-1-pentene	0	84.161	62.00	335.00	7.03E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
c-3-hexene	0.33	84.161	67.00	340.00	5.89E+00	3.60E-03	2.12E-02	0.046	2.54E-03	1	3.149E-01
3-MeCyclopentene	0	82.145	65.00	338.00	6.33E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00
1-methylcyclopentene	0.75	82.145	72.00	345.00	4.93E+00	8.39E-03	4.13E-02	0.047	4.97E-03	1	6.002E-01
3-Me-1-Hexene	0.14	98.188	84.00	357.00	3.18E+00	1.31E-03	4.17E-03	0.045	4.91E-04	1	7.085E-02
2-Methyl-2-hexene	0	98.188	95.00	368.00	2.12E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
3-ethyl-c-2-pentene	0.1	98.188	96.00	369.00	2.04E+00	9.35E-04	1.91E-03	0.045	2.24E-04	1	3.240E-02
2,3-DMe-2-Pentene	0.25	98.188	97.00	370.00	1.96E+00	2.34E-03	4.59E-03	0.045	5.40E-04	1	7.800E-02
2,4,4-Trimethyl-2-Pentene	0.09	112.21	105.00	378.00	1.45E+00	7.37E-04	1.07E-03	0.043	1.24E-04	1	2.044E-02
1-MethylCycloHexene	0	96.172	110.00	383.00	1.20E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
1-Undecene	0.04	154.29	193.00	466.00	4.15E-02	2.38E-04	9.89E-06	0.041	1.11E-06	1	2.527E-04
1-Dodecene	0.16	168.32	213.00	486.00	1.77E-02	8.73E-04	1.54E-05	0.040	1.73E-06	1	4.272E-04
OXYGENATE										1	
MTBE	6.35	88.2	55.20	328.20	8.92E+00	6.61E-02	5.90E-01	0.046	7.03E-02	1	9.119E+00
ETBE	0	102.2	70.00	343.00	5.29E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
OTHER										1	
Ethyne	0	26	-28.10	244.90	1.15E+02	0.00E+00	0.00E+00	0.073	0.00E+00	1	0.000E+00
Propyne	0	40.1	-23.00	250.00	1.01E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Propadiene	0	40.1	-34.50	238.50	1.36E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Indan	0.51	118.18	176.50	449.50	8.30E-02	3.96E-03	3.29E-04	0.043	3.80E-05	1	6.600E-03
Cyclohexene	0	82.145	83.00	356.00	3.30E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00

Diurnal Speciated Emissions

RVP (psia)	Temp (F)	Temp (R)	Temp (K)	Gasoline V.P. (psia)	Liquid MW	Vapor MW	Vapor Mr
7	105	564.6	313.56	8.10	91.85	68.00	0.049

Regular Emitter (vapor)

Compound	Liquid comp. (% by mass)	MW	Boiling pt. (deg C)	Boiling pt. (deg K)	Compound V.P. (psia)	Liquid Mole Fraction	Compound Pp (psia)	Compound Mr	Vapor Mole Fraction	Compound Specific Adj. Factor	Vapor-based speciated emissions (% by mass)
PARAFFINS											
Methane	0	16	-161.45	111.55	4.66E+02	0.00E+00	0.00E+00	0.097	0.00E+00	1	0.000E+00
Ethane	0	30.1	-88.60	184.40	4.04E+02	0.00E+00	0.00E+00	0.068	0.00E+00	1	0.000E+00
Propane	0	44.1	-42.10	230.90	1.63E+02	0.00E+00	0.00E+00	0.057	0.00E+00	1	0.000E+00
Butane	0.22	58.12	-0.50	272.50	5.37E+01	3.48E-03	1.87E-01	0.052	2.36E-02	1	2.018E+00
n-Pentane	4.01	72.15	36.07	309.07	1.71E+01	5.11E-02	8.71E-01	0.048	1.07E-01	1	1.132E+01
n-Hexane	1.8	86.18	68.73	341.73	5.54E+00	1.92E-02	1.06E-01	0.046	1.27E-02	1	1.610E+00
n-Heptane	1.21	100.75	98.43	371.43	1.86E+00	1.10E-02	2.05E-02	0.044	2.41E-03	1	3.567E-01
n-Octane	0.73	114.22	125.67	398.67	6.52E-01	5.87E-03	3.83E-03	0.043	4.43E-04	1	7.439E-02
n-Nonane	0.22	128.25	150.80	423.80	2.39E-01	1.58E-03	3.76E-04	0.042	4.31E-05	1	8.128E-03
n-Decane	0.14	142.28	174.12	447.12	9.17E-02	9.04E-04	8.29E-05	0.042	9.40E-06	1	1.967E-03
n-Undecane	0.12	156.3	195.90	468.90	3.67E-02	7.05E-04	2.59E-05	0.041	2.91E-06	1	6.698E-04
n-Dodecane	0.09	170.34	216.28	489.28	1.53E-02	4.85E-04	7.44E-06	0.040	8.32E-07	1	2.084E-04
n-Tridecane	0	184.37	235.40	508.40	6.67E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Tetradecane	0	198.4	253.70	526.70	2.97E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Pentadecane	0	212.42	268.17	541.17	1.56E-03	0.00E+00	0.00E+00	0.039	0.00E+00	1	0.000E+00
ISOPARAFFINS										1	
Isobutane	0.05	58.1	-11.70	261.30	7.40E+01	7.90E-04	5.85E-02	0.052	7.41E-03	1	6.330E-01
2,2-dimethylpropane	0	72.15	10.00	283.00	3.92E+01	0.00E+00	0.00E+00	0.048	0.00E+00	1	0.000E+00
Isopentane	8.89	72.15	27.83	300.83	2.23E+01	1.13E-01	2.53E+00	0.048	3.10E-01	1	3.285E+01
2,3-Dimethylbutane	1.98	86.18	57.98	330.98	8.10E+00	2.11E-02	1.71E-01	0.046	2.04E-02	1	2.589E+00
2-Methylpentane	3.97	86.18	60.26	333.26	7.48E+00	4.23E-02	3.16E-01	0.046	3.78E-02	1	4.792E+00
3-Methylpentane	2.19	86.18	63.27	336.27	6.73E+00	2.33E-02	1.57E-01	0.046	1.88E-02	1	2.378E+00
2,2-Dimethylpentane	0.08	100.75	79.19	352.19	3.80E+00	7.29E-04	2.77E-03	0.044	3.25E-04	1	4.815E-02
2,4-Dimethylpentane	0.41	100.75	80.49	353.49	3.62E+00	3.74E-03	1.35E-02	0.044	1.59E-03	1	2.353E-01
2,2,3-Trimethylbutane	0.03	100.75	80.88	353.88	3.57E+00	2.74E-04	9.77E-04	0.044	1.15E-04	1	1.698E-02
3,3-Dimethylpentane	0.08	100.75	86.06	359.06	2.95E+00	7.29E-04	2.15E-03	0.044	2.53E-04	1	3.742E-02
2-Methylhexane	1.59	100.75	90.05	363.05	2.55E+00	1.45E-02	3.69E-02	0.044	4.33E-03	1	6.415E-01
2,3-Dimethylpentane	0.27	100.75	91.31	364.31	2.43E+00	2.46E-03	5.98E-03	0.044	7.02E-04	1	1.039E-01
3-Methylhexane	1.4	100.75	91.84	364.84	2.38E+00	1.28E-02	3.04E-02	0.044	3.57E-03	1	5.283E-01
3-Ethylpentane	0	100.75	93.47	366.47	2.24E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
2,2-Dimethylhexane	0.27	114.22	106.84	379.84	1.35E+00	2.17E-03	2.94E-03	0.043	3.40E-04	1	5.707E-02
2,5-Dimethylhexane	0.16	114.22	109.11	382.11	1.24E+00	1.29E-03	1.59E-03	0.043	1.85E-04	1	3.101E-02
2,2,3-Trimethylpentane	0	114.22	109.84	382.84	1.21E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,4-Dimethylhexane	0.51	114.22	109.43	382.43	1.22E+00	4.10E-03	5.02E-03	0.043	5.81E-04	1	9.763E-02
2,3-Dimethylhexane	0.29	114.22	115.61	388.61	9.65E-01	2.33E-03	2.25E-03	0.043	2.60E-04	1	4.375E-02
2-Methylheptane	0.65	114.22	117.31	390.31	9.03E-01	5.23E-03	4.72E-03	0.043	5.46E-04	1	9.179E-02
4-Methylheptane	0.37	114.22	117.71	390.71	8.89E-01	2.98E-03	2.65E-03	0.043	3.06E-04	1	5.144E-02
3-Methylheptane	0.87	114.22	118.00	391.00	8.79E-01	7.00E-03	6.15E-03	0.043	7.12E-04	1	1.196E-01
3-Ethylhexane	0	114.22	118.53	391.53	8.61E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,5-Dimethylheptane	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (D)	0.37	128.25	136.00	409.00	4.33E-01	2.65E-03	1.15E-03	0.042	1.31E-04	1	2.478E-02
3,3-Dimethylheptane	0	128.25	137.01	410.01	4.16E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (L)	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethylheptane	0.05	128.25	140.50	413.50	3.62E-01	3.58E-04	1.30E-04	0.042	1.48E-05	1	2.798E-03

3,4-Dimethylheptane (D)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,4-Dimethylheptane (L)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methyloctane	0	128.25	143.26	416.26	3.24E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methyloctane	0.38	128.25	143.50	416.50	3.21E-01	2.72E-03	8.73E-04	0.042	1.00E-04	1	1.885E-02
3,3-Diethylpentane	0	128.25	147.17	420.17	2.77E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-Dimethyloctane	0.06	142.28	156.89	429.89	1.87E-01	3.87E-04	7.22E-05	0.042	8.19E-06	1	1.715E-03
3,3-Dimethyloctane	0	142.28	161.22	434.22	1.56E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethyloctane	0	142.28	164.31	437.31	1.38E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methylnonane	0	142.28	167.00	440.00	1.23E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Ethyloctane	0	142.28	167.78	440.78	1.19E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methylnonane	0	142.28	168.00	441.00	1.18E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-dimethylbutane	0.44	86.177	49.70	322.70	1.08E+01	4.69E-03	5.06E-02	0.046	6.04E-03	1	7.660E-01
2,2,4-TriMePentane	0.61	114.23	99.20	372.20	1.81E+00	4.91E-03	8.86E-03	0.043	1.03E-03	1	1.724E-01
3,3-Dimethylhexane	0.19	114.23	112.00	385.00	1.11E+00	1.53E-03	1.69E-03	0.043	1.96E-04	1	3.295E-02
2,3,4-Trimethylpentane	0.48	114.23	113.00	386.00	1.07E+00	3.86E-03	4.12E-03	0.043	4.77E-04	1	8.009E-02
2,3-MethylEthylPentane	0	114.23	116.00	389.00	9.50E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,3,5-trimethylhexane	0.05	128.26	131.00	404.00	5.28E-01	3.58E-04	1.89E-04	0.042	2.16E-05	1	4.083E-03
2,4-Dimethylheptane	0.17	128.26	133.00	406.00	4.88E-01	1.22E-03	5.94E-04	0.042	6.80E-05	1	1.283E-02
4-Methyloctane	0.48	128.26	142.00	415.00	3.41E-01	3.44E-03	1.17E-03	0.042	1.34E-04	1	2.529E-02
AROMATICS										1	
Benzene	1.42	78.11	80.09	353.09	3.67E+00	1.67E-02	6.14E-02	0.047	7.43E-03	1	8.532E-01
Toluene	7.17	92.13	110.62	383.62	1.17E+00	7.15E-02	8.36E-02	0.045	9.91E-03	1	1.342E+00
Ethylbenzene	1.04	106.16	136.19	409.19	4.30E-01	9.00E-03	3.87E-03	0.044	4.51E-04	1	7.043E-02
m-Xylene	3.34	106.16	139.10	412.10	3.83E-01	2.89E-02	1.11E-02	0.044	1.29E-03	1	2.014E-01
p-Xylene	0	106.16	138.35	411.35	3.94E-01	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
o-Xylene	1.41	106.16	144.42	417.42	3.09E-01	1.22E-02	3.77E-03	0.044	4.40E-04	1	6.870E-02
Isopropylbenzene	0.1	120.19	152.39	425.39	2.24E-01	7.64E-04	1.71E-04	0.043	1.97E-05	1	3.485E-03
n-Propylbenzene	0.52	120.19	159.22	432.22	1.70E-01	3.97E-03	6.74E-04	0.043	7.76E-05	1	1.372E-02
1-Methyl-3-Ethylbenzene	1.81	120.19	161.30	434.30	1.56E-01	1.38E-02	2.15E-03	0.043	2.48E-04	1	4.385E-02
1-Methyl-4-Ethylbenzene	0.81	120.19	161.98	434.98	1.51E-01	6.19E-03	9.37E-04	0.043	1.08E-04	1	1.908E-02
1,3,5-Trimethylbenzene	0.94	120.19	164.71	437.71	1.35E-01	7.18E-03	9.72E-04	0.043	1.12E-04	1	1.979E-02
1-Methyl-2-Ethylbenzene	0	120.19	165.15	438.15	1.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
1,2,4-Trimethylbenzene	2.72	120.19	169.34	442.34	1.12E-01	2.08E-02	2.32E-03	0.043	2.68E-04	1	4.730E-02
tert-Butylbenzene	0	134.12	169.11	442.11	1.13E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylbenzene	0.06	134.12	172.76	445.76	9.70E-02	4.11E-04	3.99E-05	0.042	4.55E-06	1	8.967E-04
sec-Butylbenzene	0.06	134.12	173.30	446.30	9.49E-02	4.11E-04	3.90E-05	0.042	4.44E-06	1	8.766E-04
1-Methyl-3-Isopropylbenzene	0	134.12	175.78	448.78	8.56E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-4-Isopropylbenzene	0.07	134.12	177.10	450.10	8.10E-02	4.79E-04	3.88E-05	0.042	4.43E-06	1	8.731E-04
1-Methyl-2-Isopropylbenzene	0	134.12	178.15	451.15	7.75E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-3-n-Propylbenzene	0.44	134.12	182.01	455.01	6.60E-02	3.01E-03	1.99E-04	0.042	2.27E-05	1	4.469E-03
1-Methyl-4-n-Propylbenzene	0.04	134.12	183.42	456.42	6.22E-02	2.74E-04	1.70E-05	0.042	1.94E-06	1	3.830E-04
n-Butylbenzene	0.07	134.12	183.27	456.27	6.26E-02	4.79E-04	3.00E-05	0.042	3.42E-06	1	6.744E-04
1,3-Dimethyl-5-Ethylbenzene	0	134.12	183.76	456.76	6.13E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2-Diethylbenzene	0.06	134.12	183.42	456.42	6.22E-02	4.11E-04	2.55E-05	0.042	2.91E-06	1	5.744E-04
1-Methyl-2-n-Propylbenzene	0.21	134.12	184.97	457.97	5.82E-02	1.44E-03	8.38E-05	0.042	9.55E-06	1	1.884E-03
1,4-Dimethyl-2-Ethylbenzene	0.39	134.12	186.83	459.83	5.39E-02	2.67E-03	1.44E-04	0.042	1.64E-05	1	3.236E-03
1,2-Dimethyl-4-Ethylbenzene	0.48	134.12	189.48	462.48	4.82E-02	3.29E-03	1.58E-04	0.042	1.81E-05	1	3.561E-03
1,3-Dimethyl-2-Ethylbenzene	0.25	134.12	190.01	463.01	4.71E-02	1.71E-03	8.06E-05	0.042	9.19E-06	1	1.814E-03
1,2-Dimethyl-3-Ethylbenzene	0	134.12	193.91	466.91	3.99E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2,4,5-Tetramethylbenzene	0.26	134.12	196.80	469.80	3.53E-02	1.78E-03	6.29E-05	0.042	7.17E-06	1	1.415E-03

2-Methylbutylbenzene	0	148.24	196.67	469.67	3.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
tert-1-Butyl-2-Methylbenzene	0	148.24	198.89	471.89	3.23E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Pentylbenzene	0	148.24	205.40	478.40	2.45E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-3,5-Dimethylbenzene	0	162.26	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-4-Ethylbenzene	0	162.26	206.11	479.11	2.37E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,3,5-Triethylbenzene	0	162.26	216.00	489.00	1.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,4-Triethylbenzene	0	162.26	217.70	490.70	1.44E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Hexylbenzene	0	162.26	226.11	499.11	1.00E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,3-TrimethylBenzene	0.67	120.19	175.00	448.00	8.84E-02	5.12E-03	4.53E-04	0.043	5.21E-05	1	9.214E-03
1,3-Diethylbenzene	0.22	134.22	181.00	454.00	6.88E-02	1.51E-03	1.04E-04	0.042	1.18E-05	1	2.331E-03
1,4-Diethylbenzene	0.85	134.22	184.00	457.00	6.07E-02	5.82E-03	3.53E-04	0.042	4.02E-05	1	7.942E-03
1,2,3,5-Tetramethylbenzene	0.39	134.22	197.90	470.90	3.37E-02	2.67E-03	9.00E-05	0.042	1.03E-05	1	2.025E-03
1,2,3,4-Tetramethylbenzene	0.18	134.22	205.00	478.00	2.49E-02	1.23E-03	3.07E-05	0.042	3.50E-06	1	6.902E-04
Amylbenzene	0	148.25	205.00	478.00	2.49E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,4-Diisopropylbenzene	0.01	162.27	203.00	476.00	2.71E-02	5.66E-05	1.54E-06	0.041	1.72E-07	1	4.113E-05
Naphthalene	0.39	128.17	218.00	491.00	1.42E-02	2.79E-03	3.98E-05	0.042	4.55E-06	1	8.581E-04
NAPTHENES										1	
Cyclopentane	0	70.13	49.26	322.26	1.09E+01	0.00E+00	0.00E+00	0.049	0.00E+00	1	0.000E+00
Methylcyclopentane	1.68	84.16	71.81	344.81	4.96E+00	1.83E-02	9.10E-02	0.046	1.09E-02	1	1.350E+00
Cyclohexane	0.52	84.16	80.72	353.72	3.59E+00	5.68E-03	2.04E-02	0.046	2.44E-03	1	3.024E-01
1,1-Dimethylcyclopentane	0	98.18	87.84	360.84	2.76E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclopentane	0.42	98.18	90.77	363.77	2.48E+00	3.93E-03	9.74E-03	0.045	1.15E-03	1	1.654E-01
trans-1,3-Dimethylcyclopentane	0	98.18	91.72	364.72	2.39E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclopentane	0.71	98.18	91.87	364.87	2.38E+00	6.64E-03	1.58E-02	0.045	1.86E-03	1	2.685E-01
Methylcyclohexane	0.84	98.18	96.01	369.01	2.04E+00	7.86E-03	1.60E-02	0.045	1.88E-03	1	2.720E-01
Ethylcyclopentane	0	98.18	103.47	376.47	1.54E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclopentane	0	112.21	109.29	382.29	1.23E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ctc-1,2,3-Trimethylcyclopentane	0	112.21	110.22	383.22	1.19E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cct-1,2,4-Trimethylcyclopentane	0	112.21	116.73	389.73	9.24E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,4-Dimethylcyclohexane	0.07	112.21	119.41	392.41	8.32E-01	5.73E-04	4.77E-04	0.043	5.53E-05	1	9.128E-03
1-Ethyl-1-Methylcyclopentane	0	112.21	121.52	394.52	7.67E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclohexane	0.17	112.21	123.42	396.42	7.12E-01	1.39E-03	9.90E-04	0.043	1.15E-04	1	1.896E-02
ccc-1,2,3-Trimethylcyclopentane	0	112.21	123.00	396.00	7.23E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
Isopropylcyclopentane	0	112.21	126.40	399.40	6.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-1,2-Dimethylcyclohexane	0.06	112.21	129.73	402.73	5.55E-01	4.91E-04	2.73E-04	0.043	3.16E-05	1	5.220E-03
n-Propylcyclopentane	0	112.21	130.95	403.95	5.29E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ccc-1,3,5-Trimethylcyclohexane	0	126.23	138.41	411.41	3.93E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,4-Trimethylcyclohexane	0	126.23	135.00	408.00	4.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctt-1,2,4-Trimethylcyclohexane	0	126.23	141.24	414.24	3.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclohexane	0	126.23	147.78	420.78	2.70E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,2-Trimethylcyclohexane	0	126.23	146.00	419.00	2.90E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclopentane	0	126.23	148.00	421.00	2.68E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isopropylcyclohexane	0	126.23	154.57	427.57	2.05E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
n-Butylcyclopentane	0	126.23	156.56	429.56	1.89E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclohexane	0	140.26	171.29	444.29	1.03E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-Propylcyclohexane	0	140.26	176.67	449.67	8.25E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-(4MP)cyclopentane	0	168.33	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclohexane	0.26	112.21	120.00	393.00	8.13E-01	2.13E-03	1.73E-03	0.043	2.01E-04	1	3.313E-02
2,2,5-Trimethylhexane	0.15	128.26	124.00	397.00	6.96E-01	1.07E-03	7.47E-04	0.042	8.55E-05	1	1.614E-02
1,1-Dimethylcyclohexane	0.25	112.21	120.00	393.00	8.13E-01	2.05E-03	1.66E-03	0.043	1.93E-04	1	3.186E-02
Ethylcyclohexane	0.07	112.21	132.00	405.00	5.08E-01	5.73E-04	2.91E-04	0.043	3.37E-05	1	5.566E-03
c-1,4-Dimethylcyclohexane	0.29	112.21	120.00	393.00	8.13E-01	2.37E-03	1.93E-03	0.043	2.24E-04	1	3.695E-02
OLEFINS										1	
Isobutene	0.04	56.11	-6.89	266.11	6.46E+01	6.55E-04	4.23E-02	0.052	5.39E-03	1	4.445E-01
1-Butene	0	56.11	-6.25	266.75	6.34E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
cis-2-Butene	0.14	56.11	3.72	276.72	4.74E+01	2.29E-03	1.09E-01	0.052	1.38E-02	1	1.140E+00

3-Methyl-1-Butene	0.08	70.13	20.06	293.06	2.87E+01	1.05E-03	3.00E-02	0.049	3.69E-03	1	3.805E-01
1-Pentene	0.25	70.13	29.97	302.97	2.09E+01	3.27E-03	6.83E-02	0.049	8.39E-03	1	8.655E-01
2-Methyl-1-Butene	0.22	70.13	31.16	304.16	2.01E+01	2.88E-03	5.78E-02	0.049	7.10E-03	1	7.325E-01
2-Methyl-1,3-Butadiene	0.02	70.13	34.00	307.00	1.83E+01	2.62E-04	4.79E-03	0.049	5.88E-04	1	6.068E-02
trans-2-Pentene	1.62	70.13	36.36	309.36	1.69E+01	2.12E-02	3.59E-01	0.049	4.41E-02	1	4.547E+00
cis-2-Pentene	0.75	70.13	36.94	309.94	1.66E+01	9.82E-03	1.63E-01	0.049	2.00E-02	1	2.064E+00
4-Methylpentene-1	0.25	84.16	53.87	326.87	9.34E+00	2.73E-03	2.55E-02	0.046	3.06E-03	1	3.782E-01
1-Hexene	0.77	84.16	63.48	336.48	6.68E+00	8.40E-03	5.61E-02	0.046	6.72E-03	1	8.323E-01
trans-2-Hexene	0.85	84.16	67.88	340.88	5.71E+00	9.28E-03	5.30E-02	0.046	6.35E-03	1	7.859E-01
2-Methylpentene-2	0.66	84.16	67.31	340.31	5.83E+00	7.20E-03	4.20E-02	0.046	5.03E-03	1	6.229E-01
cis-2-Hexene	0.54	84.16	68.88	341.88	5.51E+00	5.89E-03	3.25E-02	0.046	3.89E-03	1	4.817E-01
1-Heptene	0.12	98.19	93.64	366.64	2.23E+00	1.12E-03	2.50E-03	0.045	2.94E-04	1	4.247E-02
trans-3-Heptene	0.32	98.19	95.67	368.67	2.06E+00	2.99E-03	6.18E-03	0.045	7.27E-04	1	1.049E-01
cis-3-Heptene	0.88	98.19	95.75	368.75	2.06E+00	8.23E-03	1.69E-02	0.045	1.99E-03	1	2.878E-01
trans-2-Heptene	0.28	98.19	97.95	370.95	1.89E+00	2.62E-03	4.96E-03	0.045	5.84E-04	1	8.429E-02
cis-2-Heptene	0.43	98.19	98.41	371.41	1.86E+00	4.02E-03	7.49E-03	0.045	8.81E-04	1	1.272E-01
1-Octene	0	112.22	121.27	394.27	7.74E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-2-Octene	0	112.22	125.00	398.00	6.69E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-2-Octene	0.06	112.22	125.61	398.61	6.53E-01	4.91E-04	3.21E-04	0.043	3.72E-05	1	6.138E-03
1-Nonene	0.2	126.24	146.89	419.89	2.80E-01	1.46E-03	4.07E-04	0.042	4.67E-05	1	8.669E-03
trans-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
trans-2-Nonene	0	126.24	148.50	421.50	2.62E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-2-Nonene	0.06	126.24	148.50	421.50	2.62E-01	4.37E-04	1.14E-04	0.042	1.31E-05	1	2.437E-03
1-Decene	0	140.25	170.60	443.60	1.06E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-methylpropene	0	56.107	-6.90	266.10	6.46E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
t-2-butene	0.19	56.107	3.72	276.72	4.74E+01	3.11E-03	1.47E-01	0.052	1.88E-02	1	1.547E+00
2-methyl-2-butene	0.86	70.134	39.00	312.00	1.55E+01	1.13E-02	1.74E-01	0.049	2.14E-02	1	2.211E+00
cyclopentadiene	0.02	66.102	42.00	315.00	1.40E+01	2.78E-04	3.89E-03	0.050	4.83E-04	1	4.691E-02
cyclopentene	0.32	68.118	44.00	317.00	1.31E+01	4.31E-03	5.65E-02	0.049	6.97E-03	1	6.985E-01
3-methyl-1-pentene	0	84.161	54.00	327.00	9.30E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
4-Me-c-2-Pentene	0	84.161	57.50	330.50	8.24E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
2-methyl-1-pentene	0	84.161	62.00	335.00	7.03E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
c-3-hexene	0.33	84.161	67.00	340.00	5.89E+00	3.60E-03	2.12E-02	0.046	2.54E-03	1	3.149E-01
3-MeCyclopentene	0	82.145	65.00	338.00	6.33E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00
1-methylcyclopentene	0.75	82.145	72.00	345.00	4.93E+00	8.39E-03	4.13E-02	0.047	4.97E-03	1	6.002E-01
3-Me-1-Hexene	0.14	98.188	84.00	357.00	3.18E+00	1.31E-03	4.17E-03	0.045	4.91E-04	1	7.085E-02
2-Methyl-2-hexene	0	98.188	95.00	368.00	2.12E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
3-ethyl-c-2-pentene	0.1	98.188	96.00	369.00	2.04E+00	9.35E-04	1.91E-03	0.045	2.24E-04	1	3.240E-02
2,3-DMe-2-Pentene	0.25	98.188	97.00	370.00	1.96E+00	2.34E-03	4.59E-03	0.045	5.40E-04	1	7.800E-02
2,4,4-Trimethyl-2-Pentene	0.09	112.21	105.00	378.00	1.45E+00	7.37E-04	1.07E-03	0.043	1.24E-04	1	2.044E-02
1-MethylCycloHexene	0	96.172	110.00	383.00	1.20E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
1-Undecene	0.04	154.29	193.00	466.00	4.15E-02	2.38E-04	9.89E-06	0.041	1.11E-06	1	2.527E-04
1-Dodecene	0.16	168.32	213.00	486.00	1.77E-02	8.73E-04	1.54E-05	0.040	1.73E-06	1	4.272E-04
OXYGENATE										1	
MTBE	6.35	88.2	55.20	328.20	8.92E+00	6.61E-02	5.90E-01	0.046	7.03E-02	1	9.119E+00
ETBE	0	102.2	70.00	343.00	5.29E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
OTHER										1	
Ethyne	0	26	-28.10	244.90	1.15E+02	0.00E+00	0.00E+00	0.073	0.00E+00	1	0.000E+00
Propyne	0	40.1	-23.00	250.00	1.01E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Propadiene	0	40.1	-34.50	238.50	1.36E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Indan	0.51	118.18	176.50	449.50	8.30E-02	3.96E-03	3.29E-04	0.043	3.80E-05	1	6.600E-03
Cyclohexene	0	82.145	83.00	356.00	3.30E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00

Running Loss Speciated Emissions

RVP (psia)	Temp (F)	Temp (R)	Temp (K)	Gasoline V.P. (psia)	Liquid MW	Vapor MW	Vapor Mr
7	105	564.6	313.56	8.10	91.85	68.00	0.049

Regular Emitter (vapor)

Compound	Liquid comp. (% by mass)	MW	Boiling pt. (deg C)	Boiling pt. (deg K)	Compound V.P. (psia)	Liquid Mole Fraction	Compound Pp (psia)	Compound Mr	Vapor Mole Fraction	Compound Specific Adj. Factor	Vapor-based speciated emissions (% by mass)
PARAFFINS											
Methane	0	16	-161.45	111.55	4.66E+02	0.00E+00	0.00E+00	0.097	0.00E+00	1	0.000E+00
Ethane	0	30.1	-88.60	184.40	4.04E+02	0.00E+00	0.00E+00	0.068	0.00E+00	1	0.000E+00
Propane	0	44.1	-42.10	230.90	1.63E+02	0.00E+00	0.00E+00	0.057	0.00E+00	1	0.000E+00
Butane	0.22	58.12	-0.50	272.50	5.37E+01	3.48E-03	1.87E-01	0.052	2.36E-02	1	2.018E+00
n-Pentane	4.01	72.15	36.07	309.07	1.71E+01	5.11E-02	8.71E-01	0.048	1.07E-01	1	1.132E+01
n-Hexane	1.8	86.18	68.73	341.73	5.54E+00	1.92E-02	1.06E-01	0.046	1.27E-02	1	1.610E+00
n-Heptane	1.21	100.75	98.43	371.43	1.86E+00	1.10E-02	2.05E-02	0.044	2.41E-03	1	3.567E-01
n-Octane	0.73	114.22	125.67	398.67	6.52E-01	5.87E-03	3.83E-03	0.043	4.43E-04	1	7.439E-02
n-Nonane	0.22	128.25	150.80	423.80	2.39E-01	1.58E-03	3.76E-04	0.042	4.31E-05	1	8.128E-03
n-Decane	0.14	142.28	174.12	447.12	9.17E-02	9.04E-04	8.29E-05	0.042	9.40E-06	1	1.967E-03
n-Undecane	0.12	156.3	195.90	468.90	3.67E-02	7.05E-04	2.59E-05	0.041	2.91E-06	1	6.698E-04
n-Dodecane	0.09	170.34	216.28	489.28	1.53E-02	4.85E-04	7.44E-06	0.040	8.32E-07	1	2.084E-04
n-Tridecane	0	184.37	235.40	508.40	6.67E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Tetradecane	0	198.4	253.70	526.70	2.97E-03	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
n-Pentadecane	0	212.42	268.17	541.17	1.56E-03	0.00E+00	0.00E+00	0.039	0.00E+00	1	0.000E+00
ISOPARAFFINS										1	
Isobutane	0.05	58.1	-11.70	261.30	7.40E+01	7.90E-04	5.85E-02	0.052	7.41E-03	1	6.330E-01
2,2-dimethylpropane	0	72.15	10.00	283.00	3.92E+01	0.00E+00	0.00E+00	0.048	0.00E+00	1	0.000E+00
Isopentane	8.89	72.15	27.83	300.83	2.23E+01	1.13E-01	2.53E+00	0.048	3.10E-01	1	3.285E+01
2,3-Dimethylbutane	1.98	86.18	57.98	330.98	8.10E+00	2.11E-02	1.71E-01	0.046	2.04E-02	1	2.589E+00
2-Methylpentane	3.97	86.18	60.26	333.26	7.48E+00	4.23E-02	3.16E-01	0.046	3.78E-02	1	4.792E+00
3-Methylpentane	2.19	86.18	63.27	336.27	6.73E+00	2.33E-02	1.57E-01	0.046	1.88E-02	1	2.378E+00
2,2-Dimethylpentane	0.08	100.75	79.19	352.19	3.80E+00	7.29E-04	2.77E-03	0.044	3.25E-04	1	4.815E-02
2,4-Dimethylpentane	0.41	100.75	80.49	353.49	3.62E+00	3.74E-03	1.35E-02	0.044	1.59E-03	1	2.353E-01
2,2,3-Trimethylbutane	0.03	100.75	80.88	353.88	3.57E+00	2.74E-04	9.77E-04	0.044	1.15E-04	1	1.698E-02
3,3-Dimethylpentane	0.08	100.75	86.06	359.06	2.95E+00	7.29E-04	2.15E-03	0.044	2.53E-04	1	3.742E-02
2-Methylhexane	1.59	100.75	90.05	363.05	2.55E+00	1.45E-02	3.69E-02	0.044	4.33E-03	1	6.415E-01
2,3-Dimethylpentane	0.27	100.75	91.31	364.31	2.43E+00	2.46E-03	5.98E-03	0.044	7.02E-04	1	1.039E-01
3-Methylhexane	1.4	100.75	91.84	364.84	2.38E+00	1.28E-02	3.04E-02	0.044	3.57E-03	1	5.283E-01
3-Ethylpentane	0	100.75	93.47	366.47	2.24E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
2,2-Dimethylhexane	0.27	114.22	106.84	379.84	1.35E+00	2.17E-03	2.94E-03	0.043	3.40E-04	1	5.707E-02
2,5-Dimethylhexane	0.16	114.22	109.11	382.11	1.24E+00	1.29E-03	1.59E-03	0.043	1.85E-04	1	3.101E-02
2,2,3-Trimethylpentane	0	114.22	109.84	382.84	1.21E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,4-Dimethylhexane	0.51	114.22	109.43	382.43	1.22E+00	4.10E-03	5.02E-03	0.043	5.81E-04	1	9.763E-02
2,3-Dimethylhexane	0.29	114.22	115.61	388.61	9.65E-01	2.33E-03	2.25E-03	0.043	2.60E-04	1	4.375E-02
2-Methylheptane	0.65	114.22	117.31	390.31	9.03E-01	5.23E-03	4.72E-03	0.043	5.46E-04	1	9.179E-02
4-Methylheptane	0.37	114.22	117.71	390.71	8.89E-01	2.98E-03	2.65E-03	0.043	3.06E-04	1	5.144E-02
3-Methylheptane	0.87	114.22	118.00	391.00	8.79E-01	7.00E-03	6.15E-03	0.043	7.12E-04	1	1.196E-01
3-Ethylhexane	0	114.22	118.53	391.53	8.61E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,5-Dimethylheptane	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (D)	0.37	128.25	136.00	409.00	4.33E-01	2.65E-03	1.15E-03	0.042	1.31E-04	1	2.478E-02
3,3-Dimethylheptane	0	128.25	137.01	410.01	4.16E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,5-Dimethylheptane (L)	0	128.25	136.00	409.00	4.33E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethylheptane	0.05	128.25	140.50	413.50	3.62E-01	3.58E-04	1.30E-04	0.042	1.48E-05	1	2.798E-03

3,4-Dimethylheptane (D)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3,4-Dimethylheptane (L)	0	128.25	140.61	413.61	3.60E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methyloctane	0	128.25	143.26	416.26	3.24E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methyloctane	0.38	128.25	143.50	416.50	3.21E-01	2.72E-03	8.73E-04	0.042	1.00E-04	1	1.885E-02
3,3-Diethylpentane	0	128.25	147.17	420.17	2.77E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-Dimethyloctane	0.06	142.28	156.89	429.89	1.87E-01	3.87E-04	7.22E-05	0.042	8.19E-06	1	1.715E-03
3,3-Dimethyloctane	0	142.28	161.22	434.22	1.56E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,3-Dimethyloctane	0	142.28	164.31	437.31	1.38E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-Methylnonane	0	142.28	167.00	440.00	1.23E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Ethyloctane	0	142.28	167.78	440.78	1.19E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
3-Methylnonane	0	142.28	168.00	441.00	1.18E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2,2-dimethylbutane	0.44	86.177	49.70	322.70	1.08E+01	4.69E-03	5.06E-02	0.046	6.04E-03	1	7.660E-01
2,2,4-TriMePentane	0.61	114.23	99.20	372.20	1.81E+00	4.91E-03	8.86E-03	0.043	1.03E-03	1	1.724E-01
3,3-Dimethylhexane	0.19	114.23	112.00	385.00	1.11E+00	1.53E-03	1.69E-03	0.043	1.96E-04	1	3.295E-02
2,3,4-Trimethylpentane	0.48	114.23	113.00	386.00	1.07E+00	3.86E-03	4.12E-03	0.043	4.77E-04	1	8.009E-02
2,3-MethylEthylPentane	0	114.23	116.00	389.00	9.50E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
2,3,5-trimethylhexane	0.05	128.26	131.00	404.00	5.28E-01	3.58E-04	1.89E-04	0.042	2.16E-05	1	4.083E-03
2,4-Dimethylheptane	0.17	128.26	133.00	406.00	4.88E-01	1.22E-03	5.94E-04	0.042	6.80E-05	1	1.283E-02
4-Methyloctane	0.48	128.26	142.00	415.00	3.41E-01	3.44E-03	1.17E-03	0.042	1.34E-04	1	2.529E-02
AROMATICS										1	
Benzene	1.42	78.11	80.09	353.09	3.67E+00	1.67E-02	6.14E-02	0.047	7.43E-03	1	8.532E-01
Toluene	7.17	92.13	110.62	383.62	1.17E+00	7.15E-02	8.36E-02	0.045	9.91E-03	1	1.342E+00
Ethylbenzene	1.04	106.16	136.19	409.19	4.30E-01	9.00E-03	3.87E-03	0.044	4.51E-04	1	7.043E-02
m-Xylene	3.34	106.16	139.10	412.10	3.83E-01	2.89E-02	1.11E-02	0.044	1.29E-03	1	2.014E-01
p-Xylene	0	106.16	138.35	411.35	3.94E-01	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
o-Xylene	1.41	106.16	144.42	417.42	3.09E-01	1.22E-02	3.77E-03	0.044	4.40E-04	1	6.870E-02
Isopropylbenzene	0.1	120.19	152.39	425.39	2.24E-01	7.64E-04	1.71E-04	0.043	1.97E-05	1	3.485E-03
n-Propylbenzene	0.52	120.19	159.22	432.22	1.70E-01	3.97E-03	6.74E-04	0.043	7.76E-05	1	1.372E-02
1-Methyl-3-Ethylbenzene	1.81	120.19	161.30	434.30	1.56E-01	1.38E-02	2.15E-03	0.043	2.48E-04	1	4.385E-02
1-Methyl-4-Ethylbenzene	0.81	120.19	161.98	434.98	1.51E-01	6.19E-03	9.37E-04	0.043	1.08E-04	1	1.908E-02
1,3,5-Trimethylbenzene	0.94	120.19	164.71	437.71	1.35E-01	7.18E-03	9.72E-04	0.043	1.12E-04	1	1.979E-02
1-Methyl-2-Ethylbenzene	0	120.19	165.15	438.15	1.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
1,2,4-Trimethylbenzene	2.72	120.19	169.34	442.34	1.12E-01	2.08E-02	2.32E-03	0.043	2.68E-04	1	4.730E-02
tert-Butylbenzene	0	134.12	169.11	442.11	1.13E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylbenzene	0.06	134.12	172.76	445.76	9.70E-02	4.11E-04	3.99E-05	0.042	4.55E-06	1	8.967E-04
sec-Butylbenzene	0.06	134.12	173.30	446.30	9.49E-02	4.11E-04	3.90E-05	0.042	4.44E-06	1	8.766E-04
1-Methyl-3-Isopropylbenzene	0	134.12	175.78	448.78	8.56E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-4-Isopropylbenzene	0.07	134.12	177.10	450.10	8.10E-02	4.79E-04	3.88E-05	0.042	4.43E-06	1	8.731E-04
1-Methyl-2-Isopropylbenzene	0	134.12	178.15	451.15	7.75E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1-Methyl-3-n-Propylbenzene	0.44	134.12	182.01	455.01	6.60E-02	3.01E-03	1.99E-04	0.042	2.27E-05	1	4.469E-03
1-Methyl-4-n-Propylbenzene	0.04	134.12	183.42	456.42	6.22E-02	2.74E-04	1.70E-05	0.042	1.94E-06	1	3.830E-04
n-Butylbenzene	0.07	134.12	183.27	456.27	6.26E-02	4.79E-04	3.00E-05	0.042	3.42E-06	1	6.744E-04
1,3-Dimethyl-5-Ethylbenzene	0	134.12	183.76	456.76	6.13E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2-Diethylbenzene	0.06	134.12	183.42	456.42	6.22E-02	4.11E-04	2.55E-05	0.042	2.91E-06	1	5.744E-04
1-Methyl-2-n-Propylbenzene	0.21	134.12	184.97	457.97	5.82E-02	1.44E-03	8.38E-05	0.042	9.55E-06	1	1.884E-03
1,4-Dimethyl-2-Ethylbenzene	0.39	134.12	186.83	459.83	5.39E-02	2.67E-03	1.44E-04	0.042	1.64E-05	1	3.236E-03
1,2-Dimethyl-4-Ethylbenzene	0.48	134.12	189.48	462.48	4.82E-02	3.29E-03	1.58E-04	0.042	1.81E-05	1	3.561E-03
1,3-Dimethyl-2-Ethylbenzene	0.25	134.12	190.01	463.01	4.71E-02	1.71E-03	8.06E-05	0.042	9.19E-06	1	1.814E-03
1,2-Dimethyl-3-Ethylbenzene	0	134.12	193.91	466.91	3.99E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,2,4,5-Tetramethylbenzene	0.26	134.12	196.80	469.80	3.53E-02	1.78E-03	6.29E-05	0.042	7.17E-06	1	1.415E-03

2-Methylbutylbenzene	0	148.24	196.67	469.67	3.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
tert-1-Butyl-2-Methylbenzene	0	148.24	198.89	471.89	3.23E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Pentylbenzene	0	148.24	205.40	478.40	2.45E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-3,5-Dimethylbenzene	0	162.26	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
t-1-Butyl-4-Ethylbenzene	0	162.26	206.11	479.11	2.37E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,3,5-Triethylbenzene	0	162.26	216.00	489.00	1.55E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,4-Triethylbenzene	0	162.26	217.70	490.70	1.44E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
n-Hexylbenzene	0	162.26	226.11	499.11	1.00E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,2,3-TrimethylBenzene	0.67	120.19	175.00	448.00	8.84E-02	5.12E-03	4.53E-04	0.043	5.21E-05	1	9.214E-03
1,3-Diethylbenzene	0.22	134.22	181.00	454.00	6.88E-02	1.51E-03	1.04E-04	0.042	1.18E-05	1	2.331E-03
1,4-Diethylbenzene	0.85	134.22	184.00	457.00	6.07E-02	5.82E-03	3.53E-04	0.042	4.02E-05	1	7.942E-03
1,2,3,5-Tetramethylbenzene	0.39	134.22	197.90	470.90	3.37E-02	2.67E-03	9.00E-05	0.042	1.03E-05	1	2.025E-03
1,2,3,4-Tetramethylbenzene	0.18	134.22	205.00	478.00	2.49E-02	1.23E-03	3.07E-05	0.042	3.50E-06	1	6.902E-04
Amylbenzene	0	148.25	205.00	478.00	2.49E-02	0.00E+00	0.00E+00	0.041	0.00E+00	1	0.000E+00
1,4-Diisopropylbenzene	0.01	162.27	203.00	476.00	2.71E-02	5.66E-05	1.54E-06	0.041	1.72E-07	1	4.113E-05
Naphthalene	0.39	128.17	218.00	491.00	1.42E-02	2.79E-03	3.98E-05	0.042	4.55E-06	1	8.581E-04
NAPTHENES										1	
Cyclopentane	0	70.13	49.26	322.26	1.09E+01	0.00E+00	0.00E+00	0.049	0.00E+00	1	0.000E+00
Methylcyclopentane	1.68	84.16	71.81	344.81	4.96E+00	1.83E-02	9.10E-02	0.046	1.09E-02	1	1.350E+00
Cyclohexane	0.52	84.16	80.72	353.72	3.59E+00	5.68E-03	2.04E-02	0.046	2.44E-03	1	3.024E-01
1,1-Dimethylcyclopentane	0	98.18	87.84	360.84	2.76E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclopentane	0.42	98.18	90.77	363.77	2.48E+00	3.93E-03	9.74E-03	0.045	1.15E-03	1	1.654E-01
trans-1,3-Dimethylcyclopentane	0	98.18	91.72	364.72	2.39E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclopentane	0.71	98.18	91.87	364.87	2.38E+00	6.64E-03	1.58E-02	0.045	1.86E-03	1	2.685E-01
Methylcyclohexane	0.84	98.18	96.01	369.01	2.04E+00	7.86E-03	1.60E-02	0.045	1.88E-03	1	2.720E-01
Ethylcyclopentane	0	98.18	103.47	376.47	1.54E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclopentane	0	112.21	109.29	382.29	1.23E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ctc-1,2,3-Trimethylcyclopentane	0	112.21	110.22	383.22	1.19E+00	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cct-1,2,4-Trimethylcyclopentane	0	112.21	116.73	389.73	9.24E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,4-Dimethylcyclohexane	0.07	112.21	119.41	392.41	8.32E-01	5.73E-04	4.77E-04	0.043	5.53E-05	1	9.128E-03
1-Ethyl-1-Methylcyclopentane	0	112.21	121.52	394.52	7.67E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-1,2-Dimethylcyclohexane	0.17	112.21	123.42	396.42	7.12E-01	1.39E-03	9.90E-04	0.043	1.15E-04	1	1.896E-02
ccc-1,2,3-Trimethylcyclopentane	0	112.21	123.00	396.00	7.23E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
Isopropylcyclopentane	0	112.21	126.40	399.40	6.33E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-1,2-Dimethylcyclohexane	0.06	112.21	129.73	402.73	5.55E-01	4.91E-04	2.73E-04	0.043	3.16E-05	1	5.220E-03
n-Propylcyclopentane	0	112.21	130.95	403.95	5.29E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
ccc-1,3,5-Trimethylcyclohexane	0	126.23	138.41	411.41	3.93E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,4-Trimethylcyclohexane	0	126.23	135.00	408.00	4.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctt-1,2,4-Trimethylcyclohexane	0	126.23	141.24	414.24	3.51E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
ctc-1,2,4-Trimethylcyclohexane	0	126.23	147.78	420.78	2.70E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
1,1,2-Trimethylcyclohexane	0	126.23	146.00	419.00	2.90E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclopentane	0	126.23	148.00	421.00	2.68E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isopropylcyclohexane	0	126.23	154.57	427.57	2.05E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
n-Butylcyclopentane	0	126.23	156.56	429.56	1.89E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
Isobutylcyclohexane	0	140.26	171.29	444.29	1.03E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-Propylcyclohexane	0	140.26	176.67	449.67	8.25E-02	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
t-1-Methyl-2-(4MP)cyclopentane	0	168.33	204.44	477.44	2.55E-02	0.00E+00	0.00E+00	0.040	0.00E+00	1	0.000E+00
cis-1,3-Dimethylcyclohexane	0.26	112.21	120.00	393.00	8.13E-01	2.13E-03	1.73E-03	0.043	2.01E-04	1	3.313E-02
2,2,5-Trimethylhexane	0.15	128.26	124.00	397.00	6.96E-01	1.07E-03	7.47E-04	0.042	8.55E-05	1	1.614E-02
1,1-Dimethylcyclohexane	0.25	112.21	120.00	393.00	8.13E-01	2.05E-03	1.66E-03	0.043	1.93E-04	1	3.186E-02
Ethylcyclohexane	0.07	112.21	132.00	405.00	5.08E-01	5.73E-04	2.91E-04	0.043	3.37E-05	1	5.566E-03
c-1,4-Dimethylcyclohexane	0.29	112.21	120.00	393.00	8.13E-01	2.37E-03	1.93E-03	0.043	2.24E-04	1	3.695E-02
OLEFINS										1	
Isobutene	0.04	56.11	-6.89	266.11	6.46E+01	6.55E-04	4.23E-02	0.052	5.39E-03	1	4.445E-01
1-Butene	0	56.11	-6.25	266.75	6.34E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
cis-2-Butene	0.14	56.11	3.72	276.72	4.74E+01	2.29E-03	1.09E-01	0.052	1.38E-02	1	1.140E+00

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3-Methyl-1-Butene	0.08	70.13	20.06	293.06	2.87E+01	1.05E-03	3.00E-02	0.049	3.69E-03	1	3.805E-01
1-Pentene	0.25	70.13	29.97	302.97	2.09E+01	3.27E-03	6.83E-02	0.049	8.39E-03	1	8.655E-01
2-Methyl-1-Butene	0.22	70.13	31.16	304.16	2.01E+01	2.88E-03	5.78E-02	0.049	7.10E-03	1	7.325E-01
2-Methyl-1,3-Butadiene	0.02	70.13	34.00	307.00	1.83E+01	2.62E-04	4.79E-03	0.049	5.88E-04	1	6.068E-02
trans-2-Pentene	1.62	70.13	36.36	309.36	1.69E+01	2.12E-02	3.59E-01	0.049	4.41E-02	1	4.547E+00
cis-2-Pentene	0.75	70.13	36.94	309.94	1.66E+01	9.82E-03	1.63E-01	0.049	2.00E-02	1	2.064E+00
4-Methylpentene-1	0.25	84.16	53.87	326.87	9.34E+00	2.73E-03	2.55E-02	0.046	3.06E-03	1	3.782E-01
1-Hexene	0.77	84.16	63.48	336.48	6.68E+00	8.40E-03	5.61E-02	0.046	6.72E-03	1	8.323E-01
trans-2-Hexene	0.85	84.16	67.88	340.88	5.71E+00	9.28E-03	5.30E-02	0.046	6.35E-03	1	7.859E-01
2-Methylpentene-2	0.66	84.16	67.31	340.31	5.83E+00	7.20E-03	4.20E-02	0.046	5.03E-03	1	6.229E-01
cis-2-Hexene	0.54	84.16	68.88	341.88	5.51E+00	5.89E-03	3.25E-02	0.046	3.89E-03	1	4.817E-01
1-Heptene	0.12	98.19	93.64	366.64	2.23E+00	1.12E-03	2.50E-03	0.045	2.94E-04	1	4.247E-02
trans-3-Heptene	0.32	98.19	95.67	368.67	2.06E+00	2.99E-03	6.18E-03	0.045	7.27E-04	1	1.049E-01
cis-3-Heptene	0.88	98.19	95.75	368.75	2.06E+00	8.23E-03	1.69E-02	0.045	1.99E-03	1	2.878E-01
trans-2-Heptene	0.28	98.19	97.95	370.95	1.89E+00	2.62E-03	4.96E-03	0.045	5.84E-04	1	8.429E-02
cis-2-Heptene	0.43	98.19	98.41	371.41	1.86E+00	4.02E-03	7.49E-03	0.045	8.81E-04	1	1.272E-01
1-Octene	0	112.22	121.27	394.27	7.74E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
trans-2-Octene	0	112.22	125.00	398.00	6.69E-01	0.00E+00	0.00E+00	0.043	0.00E+00	1	0.000E+00
cis-2-Octene	0.06	112.22	125.61	398.61	6.53E-01	4.91E-04	3.21E-04	0.043	3.72E-05	1	6.138E-03
1-Nonene	0.2	126.24	146.89	419.89	2.80E-01	1.46E-03	4.07E-04	0.042	4.67E-05	1	8.669E-03
trans-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-3-Nonene	0	126.24	147.70	420.70	2.71E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
trans-2-Nonene	0	126.24	148.50	421.50	2.62E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
cis-2-Nonene	0.06	126.24	148.50	421.50	2.62E-01	4.37E-04	1.14E-04	0.042	1.31E-05	1	2.437E-03
1-Decene	0	140.25	170.60	443.60	1.06E-01	0.00E+00	0.00E+00	0.042	0.00E+00	1	0.000E+00
2-methylpropene	0	56.107	-6.90	266.10	6.46E+01	0.00E+00	0.00E+00	0.052	0.00E+00	1	0.000E+00
t-2-butene	0.19	56.107	3.72	276.72	4.74E+01	3.11E-03	1.47E-01	0.052	1.88E-02	1	1.547E+00
2-methyl-2-butene	0.86	70.134	39.00	312.00	1.55E+01	1.13E-02	1.74E-01	0.049	2.14E-02	1	2.211E+00
cyclopentadiene	0.02	66.102	42.00	315.00	1.40E+01	2.78E-04	3.89E-03	0.050	4.83E-04	1	4.691E-02
cyclopentene	0.32	68.118	44.00	317.00	1.31E+01	4.31E-03	5.65E-02	0.049	6.97E-03	1	6.985E-01
3-methyl-1-pentene	0	84.161	54.00	327.00	9.30E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
4-Me-c-2-Pentene	0	84.161	57.50	330.50	8.24E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
2-methyl-1-pentene	0	84.161	62.00	335.00	7.03E+00	0.00E+00	0.00E+00	0.046	0.00E+00	1	0.000E+00
c-3-hexene	0.33	84.161	67.00	340.00	5.89E+00	3.60E-03	2.12E-02	0.046	2.54E-03	1	3.149E-01
3-MeCyclopentene	0	82.145	65.00	338.00	6.33E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00
1-methylcyclopentene	0.75	82.145	72.00	345.00	4.93E+00	8.39E-03	4.13E-02	0.047	4.97E-03	1	6.002E-01
3-Me-1-Hexene	0.14	98.188	84.00	357.00	3.18E+00	1.31E-03	4.17E-03	0.045	4.91E-04	1	7.085E-02
2-Methyl-2-hexene	0	98.188	95.00	368.00	2.12E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
3-ethyl-c-2-pentene	0.1	98.188	96.00	369.00	2.04E+00	9.35E-04	1.91E-03	0.045	2.24E-04	1	3.240E-02
2,3-DMe-2-Pentene	0.25	98.188	97.00	370.00	1.96E+00	2.34E-03	4.59E-03	0.045	5.40E-04	1	7.800E-02
2,4,4-Trimethyl-2-Pentene	0.09	112.21	105.00	378.00	1.45E+00	7.37E-04	1.07E-03	0.043	1.24E-04	1	2.044E-02
1-MethylCycloHexene	0	96.172	110.00	383.00	1.20E+00	0.00E+00	0.00E+00	0.045	0.00E+00	1	0.000E+00
1-Undecene	0.04	154.29	193.00	466.00	4.15E-02	2.38E-04	9.89E-06	0.041	1.11E-06	1	2.527E-04
1-Dodecene	0.16	168.32	213.00	486.00	1.77E-02	8.73E-04	1.54E-05	0.040	1.73E-06	1	4.272E-04
OXYGENATE										1	
MTBE	6.35	88.2	55.20	328.20	8.92E+00	6.61E-02	5.90E-01	0.046	7.03E-02	1	9.119E+00
ETBE	0	102.2	70.00	343.00	5.29E+00	0.00E+00	0.00E+00	0.044	0.00E+00	1	0.000E+00
OTHER										1	
Ethyne	0	26	-28.10	244.90	1.15E+02	0.00E+00	0.00E+00	0.073	0.00E+00	1	0.000E+00
Propyne	0	40.1	-23.00	250.00	1.01E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Propadiene	0	40.1	-34.50	238.50	1.36E+02	0.00E+00	0.00E+00	0.059	0.00E+00	1	0.000E+00
Indan	0.51	118.18	176.50	449.50	8.30E-02	3.96E-03	3.29E-04	0.043	3.80E-05	1	6.600E-03
Cyclohexene	0	82.145	83.00	356.00	3.30E+00	0.00E+00	0.00E+00	0.047	0.00E+00	1	0.000E+00

APPENDIX C – EVAPORATIVE EMISSIONS TEST FUEL

LIQUID SPECIATION DATA

Table C-1. EPA Certification Test Fuel Liquid Composition

	Compound Name	% of Total Mass
1	Methane	
2	Ethylene	
3	Acetylene (Ethyne)	
4	Ethane	
5	Propene	
6	Propane	
7	Allene (Propadiene)	
8	Propyne	
9	2-Methylpropane	1.81
10	2-Methylpropene & 1-Butene	
11	1,3-Butadiene	
12	n-Butane	1.90
13	2,2-Dimethylpropane	
14	t-2-Butene	0.06
15	1-Butyne	
16	c-2-Butene	
17	3-Methyl-1-butene	
18	2-Methylbutane (Isopentane)	15.14
19	1-Pentene & 2-Butyne	0.00
20	2-Methyl-1-butene	0.00
21	n-Pentane	3.28
22	2-Methyl-1,3-butadiene	0.00
23	t-2-Pentene	0.00
24	3,3-Dimethyl-1-butene	
25	c-2-Pentene	
26	2-Methyl-2-butene	0.00
27	Unknown #1	
28	Cyclopentadiene	
29	2,2-Dimethylbutane	0.16
30	Cyclopentene	
31	3 & 4-Methyl-1-Pentenes	
32	Cyclopentane	0.22
33	MTBE	
34	2,3-Dimethylbutane	1.24
35	Unknown #2	
36	2-MePentane & 4-Me-c-2-Pentene	0.94
37	4-Methyl-t-2-pentene	
38	3-Methylpentane	0.51
39	2-Methyl-1-pentene & 1-Hexene	0.01

Table C-1. EPA Certification Test Fuel Liquid Composition

	Compound Name	% of Total Mass
40	n-Hexane	0.65
41	t-3-Hexene & c-3-Hexene	
42	t-2-Hexene	
43	3-Methyl-t-2-pentene	
44	2-Methyl-2-pentene	
45	c-2-Hexene & 3-MeCyclopentene	
46	ETBE	
47	3-Methyl-c-2-pentene	
48	2,2-Dimethylpentane	0.03
49	Methylcyclopentane	0.42
50	2,4-Dimethylpentane	0.88
51	2,2,3-Trimethylbutane	0.08
52	1-Methylcyclopentene	
53	Benzene	0.23
54	3,3-Dimethylpentane	0.02
55	3-Me-1-Hexene	
56	Cyclohexane	0.38
57	2-Methylhexane	0.20
58	2,3-Dimethylpentane	0.58
59	Cyclohexene & 3-Methylhexane	0.17
60	Unknown #3	
61	c-1,3-Dimethylcyclopentane	0.04
62	t-1,2-Dimethylcyclopentane	0.05
63	2,2,4-TriMePentane (IsoOctane)	12.31
64	1-Heptene	
65	t-3-Heptene	
66	n-Heptane	0.23
67	2-Methyl-2-Hexene & c-3-Heptene	
68	3-Me-t-3-Hexene & t-2-Heptene	
69	3-Ethyl-c-2-Pentene	
70	2,4,4-TMe-1- & 2,3-DMe-2-Pentene	
71	c-2-Heptene	
72	Unknown #4	
73	2,2-DiMeHexane	
74	Methylcyclohexane	0.40
75	2,4,4-Trimethyl-2-Pentene	0.03
76	2,5-DiMeHexane & EtCyPentane	1.12
77	2,4-Dimethylhexane	1.02
78	3,3-Dimethylhexane	0.02

Table C-1. EPA Certification Test Fuel Liquid Composition

	Compound Name	% of Total Mass
79	2,3,4-Trimethylpentane	6.36
80	2,3,3-Trimethylpentane	6.36
81	Toluene	22.58
82	2,3-DiMeHexane & 2,3-MeEtPentane	1.08
83	2-Methylheptane	0.07
84	1-MeCyHexene & 4-MeHeptane	0.02
85	Unknown #5	0.19
86	3-Methylheptane	0.05
87	1c-2t-3-TriMeCyPentane	0.01
88	c-1,3-Dimethylcyclohexane	0.05
89	t-1,4-Dimethylcyclohexane	0.02
90	2,2,5-Trimethylhexane	0.87
91	1-Octene	
92	1,1-Dimethylcyclohexane	0.01
93	Unknown #6	0.00
94	t-4-Octene	0.01
95	Unknown #7	0.00
96	n-Octane	0.08
97	t-2-Octene & t-1,2-DiMeCyHexane	
98	t-1,3 & c-1,4-DiMeCyHexane	0.01
99	c-2-Octene	
100	2,3,5-Trimethylhexane	0.14
101	2,4-Dimethylheptane	0.02
102	Unknown #8	0.03
103	c-1,2-Dimethylcyclohexane	
104	Ethylcyclohexane	
105	3,5-Dimethylheptane	0.06
106	Unknown #9	0.01
107	Unknown #10	0.00
108	Unknown #11	
109	Ethylbenzene	0.03
110	2-MeOctane & 2,3-DiMeHeptane	0.03
111	meta- & para-Xylenes	0.15
112	4-Methyloctane	0.02
113	3-Methyloctane	0.01
114	Unknown #12	
115	Styrene	0.01
116	Unknown #13	0.14
117	ortho-Xylene	0.25

Table C-1. EPA Certification Test Fuel Liquid Composition

	Compound Name	% of Total Mass
118	1-Nonene	0.09
119	c- & t-4-Nonene	0.01
120	n-Nonane	0.06
121	t-2-Nonene	0.05
122	Isopropylbenzene (Cumene)	0.13
123	2,2-Dimethyloctane	0.03
124	Unknown #14	0.02
125	2,4-DiMeOctane+AlBenz+PrCyHexane	0.08
126	Unknown #15	0.01
127	n-Propylbenzene	0.65
128	1-Methyl-3-Ethylbenzene	2.62
129	1-Methyl-4-Ethylbenzene	1.19
130	1,3,5-Trimethylbenzene	1.39
131	Unknown #16	0.26
132	Unknown #17	
133	1-Ethyl-2-Methylbenzene	1.01
134	3-Methylnonane	
135	1,2,4-TriMeBenz & t-Butylbenzene	4.51
136	n-Decane	0.19
137	Isobutylbenzene	0.06
138	sec-Butylbenzene	0.08
139	1-Methyl-4-Isobutylbenzene	0.11
140	1,2,3-Trimethylbenzene	0.76
141	4-Isopropyltoluene (p-Cymene)	0.04
142	Indan	0.36
143	1,3-Diethylbenzene	0.12
144	1-Methyl-3-Propylbenzene	0.54
145	1,4-Diethylbenzene	0.32
146	1,2-Diethylbenzene	0.03
147	n-Butylbenzene	
148	1-Methyl-2-Propylbenzene	0.04
149	1,4-Dimethyl-2-Ethylbenzene	0.07
150	1,3-Dimethyl-4-Ethylbenzene	0.06
151	1,2-Dimethyl-4-Ethylbenzene	0.08
152	1,3-Dimethyl-2-Ethylbenzene	0.13
153	1-Undecene	
154	n-Undecane	0.02
155	Unknown #18	0.03
156	Unknown #19	

Table C-1. EPA Certification Test Fuel Liquid Composition

	Compound Name	% of Total Mass
157	1,2,4,5-Tetramethylbenzene	0.02
158	1,2,3,5-Tetramethylbenzene	0.03
159	Unknown #20	0.01
160	Unknown #21	
161	Methylindan	0.01
162	1,3-Diisopropylbenzene	0.02
163	1,2,3,4-TetMeBenzene & Amylbenz	0.01
164	Unknown #22	0.00
165	Unknown #23	
166	1,4-Diisopropylbenzene	0.00
167	Unknown #24	0.00
168	Naphthalene	0.15
169	1-Dodecene	0.00
170	Unknown #25	0.01
171	Unknown #26	0.00
172	n-Dodecane	0.01
	Others	1.71
	Total	100.00

Table C-2. Houston Texas Summer Ozone Season Reformulated Fuel Liquid Composition

	Compound Name	% of Total Mass
1	Methane	
2	Ethylene	
3	Acetylene (Ethyne)	
4	Ethane	
5	Propene	
6	Propane	
7	Allene (Propadiene)	
8	Propyne	
9	2-Methylpropane	0.05
10	2-Methylpropene & 1-Butene	0.04
11	1,3-Butadiene	
12	n-Butane	0.22
13	2,2-Dimethylpropane	
14	t-2-Butene	0.19
15	1-Butyne	
16	c-2-Butene	0.14
17	3-Methyl-1-butene	0.08
18	2-Methylbutane (Isopentane)	8.89
19	1-Pentene & 2-Butyne	0.25
20	2-Methyl-1-butene	0.22
21	n-Pentane	4.01
22	2-Methyl-1,3-butadiene	0.02
23	t-2-Pentene	1.62
24	3,3-Dimethyl-1-butene	
25	c-2-Pentene	0.75
26	2-Methyl-2-butene	0.86
27	Unknown #1	0.03
28	Cyclopentadiene	0.02
29	2,2-Dimethylbutane	0.44
30	Cyclopentene	0.32
31	3 & 4-Methyl-1-Pentenes	0.25
32	Cyclopentane	
33	MTBE	6.35
34	2,3-Dimethylbutane	1.98
35	Unknown #2	
36	2-MePentane & 4-Me-c-2-Pentene	3.97
37	4-Methyl-t-2-pentene	

Table C-2. Houston Texas Summer Ozone Season Reformulated Fuel Liquid Composition

	Compound Name	% of Total Mass
38	3-Methylpentane	2.19
39	2-Methyl-1-pentene & 1-Hexene	0.77
40	n-Hexane	1.80
41	t-3-Hexene & c-3-Hexene	0.33
42	t-2-Hexene	0.85
43	3-Methyl-t-2-pentene	0.68
44	2-Methyl-2-pentene	0.66
45	c-2-Hexene & 3-MeCyclopentene	0.54
46	ETBE	
47	3-Methyl-c-2-pentene	0.69
48	2,2-Dimethylpentane	0.08
49	Methylcyclopentane	1.68
50	2,4-Dimethylpentane	0.41
51	2,2,3-Trimethylbutane	0.03
52	1-Methylcyclopentene	0.75
53	Benzene	1.42
54	3,3-Dimethylpentane	0.08
55	3-Me-1-Hexene	0.14
56	Cyclohexane	0.52
57	2-Methylhexane	1.59
58	2,3-Dimethylpentane	0.27
59	Cyclohexene & 3-Methylhexane	1.40
60	Unknown #3	0.08
61	c-1,3-Dimethylcyclopentane	0.42
62	t-1,2-Dimethylcyclopentane	0.71
63	2,2,4-TriMePentane (IsoOctane)	0.61
64	1-Heptene	0.12
65	t-3-Heptene	0.32
66	n-Heptane	1.21
67	2-Methyl-2-Hexene & c-3-Heptene	0.88
68	3-Me-t-3-Hexene & t-2-Heptene	0.28
69	3-Ethyl-c-2-Pentene	0.10
70	2,4,4-TMe-1- & 2,3-DMe-2-Pentene	0.25
71	c-2-Heptene	0.43
72	Unknown #4	0.08
73	2,2-DiMeHexane	0.27
74	Methylcyclohexane	0.84
75	2,4,4-Trimethyl-2-Pentene	0.09

Table C-2. Houston Texas Summer Ozone Season Reformulated Fuel Liquid Composition

	Compound Name	% of Total Mass
76	2,5-DiMeHexane & EtCyPentane	0.16
77	2,4-Dimethylhexane	0.51
78	3,3-Dimethylhexane	0.19
79	2,3,4-Trimethylpentane	0.48
80	2,3,3-Trimethylpentane	0.48
81	Toluene	7.17
82	2,3-DiMeHexane & 2,3-MeEtPentane	0.29
83	2-Methylheptane	0.65
84	1-MeCyHexene & 4-MeHeptane	0.37
85	Unknown #5	0.10
86	3-Methylheptane	0.87
87	1c-2t-3-TriMeCyPentane	
88	c-1,3-Dimethylcyclohexane	0.26
89	t-1,4-Dimethylcyclohexane	0.07
90	2,2,5-Trimethylhexane	0.15
91	1-Octene	
92	1,1-Dimethylcyclohexane	0.25
93	Unknown #6	0.13
94	t-4-Octene	0.27
95	Unknown #7	0.23
96	n-Octane	0.73
97	t-2-Octene & t-1,2-DiMeCyHexane	0.17
98	t-1,3 & c-1,4-DiMeCyHexane	0.29
99	c-2-Octene	0.06
100	2,3,5-Trimethylhexane	0.05
101	2,4-Dimethylheptane	0.17
102	Unknown #8	0.09
103	c-1,2-Dimethylcyclohexane	0.06
104	Ethylcyclohexane	0.07
105	3,5-Dimethylheptane	0.37
106	Unknown #9	0.05
107	Unknown #10	0.15
108	Unknown #11	0.07
109	Ethylbenzene	1.04
110	2-MeOctane & 2,3-DiMeHeptane	0.05
111	meta- & para-Xylenes	3.34
112	4-Methyloctane	0.48
113	3-Methyloctane	0.38

Table C-2. Houston Texas Summer Ozone Season Reformulated Fuel Liquid Composition

	Compound Name	% of Total Mass
114	Unknown #12	0.03
115	Styrene	0.02
116	Unknown #13	0.07
117	ortho-Xylene	1.41
118	1-Nonene	0.20
119	c- & t-4-Nonene	0.12
120	n-Nonane	0.22
121	t-2-Nonene	0.06
122	Isopropylbenzene (Cumene)	0.10
123	2,2-Dimethyloctane	0.06
124	Unknown #14	0.09
125	2,4-DiMeOctane+AlBenz+PrCyHexane	0.20
126	Unknown #15	0.04
127	n-Propylbenzene	0.52
128	1-Methyl-3-Ethylbenzene	1.81
129	1-Methyl-4-Ethylbenzene	0.81
130	1,3,5-Trimethylbenzene	0.94
131	Unknown #16	0.19
132	Unknown #17	0.03
133	1-Ethyl-2-Methylbenzene	0.81
134	3-Methylnonane	
135	1,2,4-TriMeBenz & t-Butylbenzene	2.72
136	n-Decane	0.14
137	Isobutylbenzene	0.06
138	sec-Butylbenzene	0.06
139	1-Methyl-4-Isobutylbenzene	0.07
140	1,2,3-Trimethylbenzene	0.67
141	4-Isopropyltoluene (p-Cymene)	0.04
142	Indan	0.51
143	1,3-Diethylbenzene	0.22
144	1-Methyl-3-Propylbenzene	0.44
145	1,4-Diethylbenzene	0.85
146	1,2-Diethylbenzene	0.06
147	n-Butylbenzene	0.07
148	1-Methyl-2-Propylbenzene	0.21
149	1,4-Dimethyl-2-Ethylbenzene	0.39
150	1,3-Dimethyl-4-Ethylbenzene	0.27
151	1,2-Dimethyl-4-Ethylbenzene	0.48

Table C-2. Houston Texas Summer Ozone Season Reformulated Fuel Liquid Composition

	Compound Name	% of Total Mass
152	1,3-Dimethyl-2-Ethylbenzene	0.25
153	1-Undecene	0.04
154	n-Undecane	0.12
155	Unknown #18	0.15
156	Unknown #19	0.03
157	1,2,4,5-Tetramethylbenzene	0.26
158	1,2,3,5-Tetramethylbenzene	0.39
159	Unknown #20	0.12
160	Unknown #21	
161	Methylindan	0.50
162	1,3-Diisopropylbenzene	0.56
163	1,2,3,4-TetMeBenzene & Amylbenz	0.18
164	Unknown #22	0.16
165	Unknown #23	0.27
166	1,4-Diisopropylbenzene	0.01
167	Unknown #24	0.14
168	Naphthalene	0.39
169	1-Dodecene	0.19
170	Unknown #25	0.16
171	Unknown #26	0.17
172	n-Dodecane	0.09
	Others	6.32
	Total	100.00

APPENDIX D - EVAPORATIVE EMISSIONS EXPERIMENTS 2-8:

MEASURED vs. MODEL-PREDICTED SPECIATION RESULTS

Table D-1. Measured vs TEVAP-Predicted Speciation Profiles: Expt.2 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	50.47	43.88	1.15
Isobutane	17.20	17.98	0.96
n-Pentane	9.38	7.26	1.29
Butane	8.44	13.67	0.62
2,2,4-TriMePentane	2.86	2.73	1.05
Toluene	2.23	3.32	0.67
2,3-Dimethylbutane	2.21	1.27	1.74
2-Methylpentane	1.27	0.89	1.43
2,3,4-Trimethylpentane	0.70	0.83	0.84
3-Methylpentane	0.60	0.43	1.37
n-Hexane	0.59	0.46	1.30
2,4-Dimethylpentane	0.50	0.40	1.27
t-2-butene	0.38	0.38	1.00
Methylcyclopentane	0.31	0.26	1.17
2,2-dimethylbutane	0.31	0.22	1.41
Propane	0.27	0.00	
2,4-Dimethylhexane	0.22	0.15	1.43
2,3-Dimethylhexane	0.19	0.13	1.49
Cyclohexane	0.18	0.17	1.03
2,5-Dimethylhexane	0.14	0.17	0.85
Total	98.47	94.61	
Average			1.04

Table D-2. Measured vs TEVAP-Predicted Speciation Profiles: Expt.2 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	47.01	43.88	1.07
Isobutane	13.53	17.98	0.75
n-Pentane	9.40	7.26	1.29
Butane	7.13	13.67	0.52
2,2,4-TriMePentane	5.92	2.73	2.17
Toluene	4.18	3.32	1.26
2,3-Dimethylbutane	2.36	1.27	1.86
2-Methylpentane	1.37	0.89	1.54
2,3,4-Trimethylpentane	1.35	0.83	1.63
n-Hexane	0.72	0.46	1.59
2,4-Dimethylpentane	0.71	0.40	1.80
3-Methylpentane	0.67	0.43	1.53
2,4-Dimethylhexane	0.49	0.15	3.19
Methylcyclopentane	0.43	0.26	1.62
2,3-Dimethylpentane	0.36	0.18	2.06
2,5-Dimethylhexane	0.32	0.17	1.89
2,2-dimethylbutane	0.31	0.22	1.43
Cyclohexane	0.31	0.17	1.79
t-2-butene	0.30	0.38	0.78
Benzene	0.23	0.11	2.12
Total	97.13	94.77	
Average			1.02

Table D-3. Measured vs TEVAP-Predicted Speciation Profiles: Expt.2 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	36.96	43.32	0.85
Isobutane	26.63	19.07	1.40
Butane	11.45	14.21	0.81
n-Pentane	6.46	7.06	0.92
Toluene	5.82	2.81	2.07
2,2,4-TriMePentane	3.17	2.36	1.34
2,3-Dimethylbutane	1.32	1.19	1.11
2,3,4-Trimethylpentane	1.08	0.70	1.53
2-Methylpentane	0.86	0.83	1.04
Propane	0.52	0.00	
n-Hexane	0.47	0.42	1.12
3-Methylpentane	0.43	0.40	1.08
t-2-butene	0.43	0.40	1.08
2,4-Dimethylpentane	0.40	0.36	1.12
Methylcyclopentane	0.27	0.24	1.10
2,5-Dimethylhexane	0.21	0.14	1.46
2,3-Dimethylpentane	0.19	0.15	1.25
2,2-dimethylbutane	0.19	0.21	0.89
Cyclopentane	0.17	0.30	0.58
Cyclohexane	0.17	0.16	1.09
Total	97.20	94.34	
Average			1.03

Table D-4. Measured vs TEVAP-Predicted Speciation Profiles: Expt.3 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	49.44	43.58	1.13
Isobutane	18.99	18.64	1.02
n-Pentane	9.02	7.15	1.26
Butane	8.88	14.01	0.63
Toluene	2.54	3.01	0.85
2,2,4-TriMePentane	2.37	2.51	0.94
2,3-Dimethylbutane	1.70	1.22	1.39
2-Methylpentane	1.13	0.85	1.32
2,3,4-Trimethylpentane	0.76	0.75	1.00
3-Methylpentane	0.52	0.42	1.25
n-Hexane	0.50	0.43	1.15
2,4-Dimethylpentane	0.40	0.37	1.07
Propane	0.35	0.00	
t-2-butene	0.35	0.39	0.90
2,2-dimethylbutane	0.28	0.21	1.34
Cyclopentane	0.28	0.30	0.92
Methylcyclopentane	0.25	0.25	1.01
2,3-Dimethylpentane	0.15	0.16	0.91
2,5-Dimethylhexane	0.15	0.15	0.95
2,4-Dimethylhexane	0.15	0.14	1.05
Total	98.20	94.56	
Average			1.04

Table D-5. Measured vs TEVAP-Predicted Speciation Profiles: Expt.3 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	48.64	43.58	1.12
Isobutane	13.60	18.64	0.73
n-Pentane	8.77	7.15	1.23
Butane	6.86	14.01	0.49
Toluene	6.34	3.01	2.11
2,2,4-TriMePentane	3.74	2.51	1.49
2,3-Dimethylbutane	1.98	1.22	1.62
2-Methylpentane	1.30	0.85	1.52
2,3,4-Trimethylpentane	1.22	0.75	1.61
n-Hexane	0.66	0.43	1.53
3-Methylpentane	0.63	0.42	1.52
2,4-Dimethylpentane	0.57	0.37	1.53
Methylcyclopentane	0.38	0.25	1.54
2,2-dimethylbutane	0.29	0.21	1.37
Cyclopentane	0.29	0.30	0.95
t-2-butene	0.28	0.39	0.73
2,3-Dimethylpentane	0.26	0.16	1.63
Cyclohexane	0.26	0.16	1.59
2,4-Dimethylhexane	0.24	0.14	1.72
2,5-Dimethylhexane	0.23	0.15	1.49
Total	96.53	94.72	
Average			1.02

Table D-6. Measured vs TEVAP-Predicted Speciation Profiles: Expt. 3 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	35.24	43.10	0.82
Isobutane	24.88	19.37	1.28
Butane	10.75	14.35	0.75
Toluene	6.80	2.68	2.53
n-Pentane	5.95	7.00	0.85
2,2,4-TriMePentane	4.97	2.27	2.19
2,3,4-Trimethylpentane	1.40	0.67	2.08
2,3-Dimethylbutane	1.36	1.16	1.16
2-Methylpentane	0.89	0.81	1.10
2,4-Dimethylpentane	0.59	0.34	1.72
n-Hexane	0.57	0.41	1.39
3-Methylpentane	0.47	0.39	1.20
Propane	0.46	0.00	
t-2-butene	0.41	0.40	1.02
Methylcyclopentane	0.38	0.23	1.61
2,3-Dimethylpentane	0.33	0.15	2.21
Cyclohexane	0.30	0.15	1.97
2,4-Dimethylhexane	0.28	0.12	2.24
2,5-Dimethylhexane	0.28	0.14	1.99
Benzene	0.25	0.09	2.61
Total	96.54	93.84	
Average			1.03

Table D-7. Measured vs TEVAP-Predicted Speciation Profiles: Expt.4 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	51.66	43.88	1.18
Isobutane	14.89	17.98	0.83
Butane	8.34	13.67	0.61
n-Pentane	7.80	7.26	1.07
2,2,4-TriMePentane	4.00	2.73	1.47
Toluene	2.72	3.32	0.82
2,3-Dimethylbutane	1.92	1.27	1.51
2-Methylpentane	1.32	0.89	1.48
2,3,4-Trimethylpentane	0.97	0.83	1.17
n-Hexane	0.65	0.46	1.43
3-Methylpentane	0.63	0.43	1.45
2,4-Dimethylpentane	0.58	0.40	1.48
Methylcyclopentane	0.36	0.26	1.37
t-2-butene	0.35	0.38	0.90
2,4-Dimethylhexane	0.32	0.15	2.11
2,2-dimethylbutane	0.31	0.22	1.43
Propane	0.30	0.00	
2,3-Dimethylpentane	0.26	0.18	1.47
Cyclohexane	0.23	0.17	1.34
2,5-Dimethylhexane	0.21	0.17	1.23
Total	97.83	94.66	
Average			1.03

Table D-8. Measured vs TEVAP-Predicted Speciation Profiles: Expt.4 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	46.63	43.88	1.06
Isobutane	13.64	17.98	0.76
n-Pentane	8.69	7.26	1.20
Butane	7.00	13.67	0.51
2,2,4-TriMePentane	5.54	2.73	2.03
Toluene	5.19	3.32	1.57
2,3-Dimethylbutane	1.93	1.27	1.52
2,3,4-Trimethylpentane	1.61	0.83	1.94
2-Methylpentane	1.29	0.89	1.45
n-Hexane	0.69	0.46	1.51
2,4-Dimethylpentane	0.67	0.40	1.70
3-Methylpentane	0.63	0.43	1.45
2,4-Dimethylhexane	0.53	0.15	3.47
Methylcyclopentane	0.42	0.26	1.58
2,3-Dimethylpentane	0.34	0.18	1.97
2,5-Dimethylhexane	0.34	0.17	2.02
Cyclohexane	0.30	0.17	1.74
2,2-dimethylbutane	0.29	0.22	1.33
Cyclopentane	0.29	0.00	
t-2-butene	0.29	0.38	0.75
Total	96.33	94.66	
Average			1.02

Table D-9. Measured vs TEVAP-Predicted Speciation Profiles: Expt.4 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	32.67	43.32	0.75
Isobutane	24.06	19.07	1.26
Butane	11.08	14.21	0.78
n-Pentane	7.48	7.06	1.06
Toluene	7.01	2.81	2.49
2,2,4-TriMePentane	5.41	2.36	2.29
2,3,4-Trimethylpentane	1.88	0.70	2.68
2,3-Dimethylbutane	1.19	1.19	1.00
2-Methylpentane	0.82	0.83	0.99
2,4-Dimethylhexane	0.58	0.13	4.42
2,4-Dimethylpentane	0.54	0.36	1.51
n-Hexane	0.51	0.42	1.21
t-2-butene	0.44	0.40	1.12
3-Methylpentane	0.43	0.40	1.06
Propane	0.40	0.00	
2,5-Dimethylhexane	0.36	0.14	2.51
Methylcyclopentane	0.34	0.24	1.40
2,3-Dimethylpentane	0.32	0.15	2.06
2,3-Dimethylhexane	0.28	0.11	2.57
Cyclohexane	0.27	0.16	1.71
Total	96.05	94.07	
Average			1.02

Table D-10. Measured vs TEVAP-Predicted Speciation Profiles: Expt.5 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	46.32	43.58	1.06
Isobutane	17.86	18.64	0.96
Butane	8.05	14.01	0.57
n-Pentane	8.02	7.15	1.12
2,3-Dimethylbutane	2.87	1.22	2.35
2,2,4-TriMePentane	2.35	2.51	0.94
2-Methylpentane	1.73	0.85	2.02
Toluene	1.59	3.01	0.53
n-Hexane	0.93	0.43	2.15
3-Methylpentane	0.89	0.42	2.14
m-Xylene	0.65	0.01	104.05
2,3,4-Trimethylpentane	0.62	0.75	0.82
2,4-Dimethylpentane	0.54	0.37	1.44
Methylcyclopentane	0.53	0.25	2.10
Propane	0.37	0.00	
t-2-butene	0.34	0.39	0.86
2-Methylhexane	0.32	0.06	5.43
2,2-dimethylbutane	0.31	0.21	1.47
2,3-Dimethylpentane	0.28	0.16	1.75
3-Methylhexane	0.28	0.05	6.09
Total	94.86	94.07	
Average			1.01

Table D-11. Measured vs TEVAP-Predicted Speciation Profiles: Expt.5 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	43.39	43.58	1.00
Isobutane	14.44	18.64	0.77
n-Pentane	7.84	7.15	1.10
Butane	6.88	14.01	0.49
Toluene	3.07	3.01	1.02
2,3-Dimethylbutane	2.93	1.22	2.40
2,2,4-TriMePentane	2.73	2.51	1.09
2-Methylpentane	1.63	0.85	1.91
m-Xylene	1.03	0.01	164.35
n-Hexane	0.93	0.43	2.14
3-Methylpentane	0.84	0.42	2.02
2,3,4-Trimethylpentane	0.71	0.75	0.95
Benzene	0.61	0.10	5.98
Methylcyclopentane	0.56	0.25	2.25
2,4-Dimethylpentane	0.55	0.37	1.47
1,2,4-Trimethylbenzene	0.39	0.05	7.49
2-Methylhexane	0.39	0.06	6.62
3-Methylhexane	0.35	0.05	7.41
o-Xylene	0.34	0.01	40.58
Propane	0.33	0.00	
Total	89.93	93.47	
Average			0.96

Table D-12. Measured vs TEVAP-Predicted Speciation Profiles: Expt.5 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	40.99	43.10	0.95
Isobutane	26.68	19.37	1.38
Butane	9.43	14.35	0.66
n-Pentane	6.38	7.00	0.91
Toluene	3.00	2.68	1.12
2,3-Dimethylbutane	1.94	1.16	1.66
2,2,4-TriMePentane	1.86	2.27	0.82
2-Methylpentane	0.99	0.81	1.22
Propane	0.61	0.00	
3-Methylpentane	0.51	0.39	1.29
n-Hexane	0.46	0.41	1.12
t-2-butene	0.40	0.40	1.01
Benzene	0.40	0.09	4.25
2,3,4-Trimethylpentane	0.39	0.67	0.59
Methylcyclopentane	0.36	0.23	1.52
2,4-Dimethylpentane	0.34	0.34	0.99
m-Xylene	0.21	0.01	39.56
2,2-dimethylbutane	0.21	0.20	1.01
2-Methylhexane	0.19	0.05	3.51
2,3-Dimethylpentane	0.18	0.15	1.25
Total	95.53	93.69	
Average			1.02

Table D-13. Measured vs TEVAP-Predicted Speciation Profiles: Expt.6 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	48.85	32.81	1.49
n-Pentane	9.92	11.20	0.89
MTBE	5.38	8.84	0.61
Butane	2.70	2.08	1.30
2-Methylpentane	2.54	4.62	0.55
Toluene	2.50	1.22	2.04
2,2,4-TriMePentane	2.15	0.16	13.53
t-2-butene	1.54	1.59	0.97
trans-2-Pentene	1.41	4.50	0.31
3-Methylpentane	1.27	2.28	0.56
n-Hexane	1.09	1.54	0.71
cis-2-Butene	1.06	1.17	0.90
Isobutane	1.00	0.66	1.51
m-Xylene	0.98	0.18	5.51
2,3,4-Trimethylpentane	0.80	0.07	10.96
Methylcyclopentane	0.69	1.28	0.54
Benzene	0.63	0.80	0.78
cis-2-Pentene	0.60	2.04	0.29
1-Butene	0.56	0.00	
2,2-dimethylbutane	0.49	0.75	0.65
Total	86.15	77.80	
Average			1.11

Table D-14. Measured vs TEVAP-Predicted Speciation Profiles: Expt.6 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Toluene	14.47	1.22	11.81
Isopentane	13.33	32.81	0.41
MTBE	7.64	8.84	0.86
n-Pentane	5.25	11.20	0.47
m-Xylene	4.44	0.18	24.94
Benzene	3.40	0.80	4.23
2-Methylpentane	2.86	4.62	0.62
trans-2-Pentene	2.38	4.50	0.53
1,2,4-Trimethylbenzene	2.36	0.04	58.33
o-Xylene	1.70	0.06	28.06
1-Methyl-3-Ethylbenzene	1.61	0.04	42.44
n-Hexane	1.57	1.54	1.02
3-Methylpentane	1.47	2.28	0.64
Methylcyclopentane	1.33	1.28	1.03
Ethylbenzene	1.29	0.06	20.63
2-methyl-2-butene	1.10	2.18	0.51
cis-2-Pentene	1.04	2.04	0.51
2-Methylhexane	0.93	0.60	1.55
trans-2-Hexene	0.91	0.75	1.21
3-Methylhexane	0.84	0.49	1.72
Total	69.91	75.55	
Average			0.93

Table D-15. Measured vs TEVAP-Predicted Speciation Profiles: Expt.6 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	20.56	32.65	0.63
MTBE	10.67	8.50	1.26
n-Pentane	8.31	11.04	0.75
Toluene	8.11	1.10	7.37
2-Methylpentane	4.16	4.42	0.94
trans-2-Pentene	3.71	4.43	0.84
Benzene	2.65	0.75	3.54
3-Methylpentane	2.09	2.18	0.96
n-Hexane	1.91	1.45	
2-methyl-2-butene	1.80	2.14	0.84
m-Xylene	1.65	0.15	10.71
cis-2-Pentene	1.64	2.01	0.82
Methylcyclopentane	1.57	1.21	1.29
Butane	1.25	2.14	0.58
trans-2-Hexene	1.04	0.71	1.46
t-2-butene	0.99	1.63	0.61
2-Methylhexane	0.98	0.55	1.77
1-Hexene	0.95	0.76	1.25
3-Methylhexane	0.85	0.45	1.89
1-methylcyclopentene	0.85	0.54	1.57
Total	75.73	78.82	
Average			0.96

Table D-16. Measured vs TEVAP-Predicted Speciation Profiles: Expt.7 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	27.34	32.81	0.83
n-Pentane	12.18	11.20	1.09
MTBE	12.17	8.84	1.38
2-Methylpentane	5.54	4.62	1.20
trans-2-Pentene	4.61	4.50	1.02
3-Methylpentane	2.73	2.28	1.20
2-methyl-2-butene	2.21	2.18	1.01
cis-2-Pentene	2.07	2.04	1.01
Butane	1.83	2.08	0.88
n-Hexane	1.82	1.54	1.19
Toluene	1.71	1.22	1.40
Methylcyclopentane	1.49	1.28	1.16
t-2-butene	1.41	1.59	0.89
Benzene	1.06	0.80	1.32
cis-2-Butene	0.98	1.17	0.84
1-Hexene	0.91	0.80	1.14
2,2-dimethylbutane	0.88	0.75	1.18
Cyclopentane	0.87	0.00	
2,3-Dimethylbutane	0.87	2.50	0.35
trans-2-Hexene	0.83	0.75	1.11
Total	83.53	82.96	
Average			1.01

Table D-17. Measured vs TEVAP-Predicted Speciation Profiles: Expt.7 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	24.02	32.81	0.73
Butane	19.80	2.08	9.52
MTBE	8.88	8.84	1.00
n-Pentane	8.34	11.20	0.74
2-Methylpentane	3.92	4.62	0.85
trans-2-Pentene	3.21	4.50	0.71
Toluene	2.78	1.22	2.27
3-Methylpentane	1.96	2.28	0.86
2-methyl-2-butene	1.58	2.18	0.72
cis-2-Pentene	1.41	2.04	0.69
n-Hexane	1.39	1.54	0.90
Methylcyclopentane	1.17	1.28	0.91
Benzene	1.12	0.80	1.39
t-2-butene	0.84	1.59	0.53
Isobutane	0.83	0.66	1.26
1-Hexene	0.70	0.80	0.88
trans-2-Hexene	0.66	0.75	0.88
cis-2-Butene	0.65	1.17	0.56
2,3-Dimethylbutane	0.64	2.50	0.25
2-Methylhexane	0.63	0.60	1.05
Total	84.53	83.47	
Average			1.01

Table D-18. Measured vs TEVAP-Predicted Speciation Profiles: Expt.7 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	34.23	32.65	1.05
n-Pentane	11.65	11.04	1.06
MTBE	10.83	8.50	1.27
2-Methylpentane	4.90	4.42	1.11
trans-2-Pentene	4.38	4.43	0.99
3-Methylpentane	2.38	2.18	1.10
2-methyl-2-butene	2.05	2.14	0.96
cis-2-Pentene	1.93	2.01	0.96
Butane	1.90	2.14	0.89
n-Hexane	1.58	1.45	1.09
Toluene	1.57	1.10	1.43
t-2-butene	1.42	1.63	0.87
Methylcyclopentane	1.26	1.21	1.04
cis-2-Butene	1.01	1.20	0.84
Benzene	0.89	0.75	1.19
2,2-dimethylbutane	0.81	0.72	1.12
1-Hexene	0.80	0.76	1.05
1-Pentene	0.79	0.86	0.93
Cyclopentane	0.78	0.00	
2,3-Dimethylbutane	0.78	2.40	0.32
Total	85.95	81.59	
Average			1.05

Table D-19. Measured vs TEVAP-Predicted Speciation Profiles: Expt.8 Running Loss Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	35.88	32.85	1.09
n-Pentane	12.54	11.32	1.11
2-Methylpentane	6.00	4.79	1.25
trans-2-Pentene	4.76	4.55	1.05
3-Methylpentane	2.98	2.38	1.25
2-methyl-2-butene	2.32	2.21	1.05
cis-2-Pentene	2.15	2.06	1.04
Toluene	2.11	1.34	1.57
n-Hexane	2.03	1.61	1.26
Butane	1.88	2.02	0.93
Methylcyclopentane	1.65	1.35	1.23
t-2-butene	1.43	1.55	0.92
Benzene	1.17	0.85	1.37
cis-2-Butene	1.03	1.14	0.91
2,3-Dimethylbutane	1.02	2.59	0.40
1-Hexene	1.01	0.83	1.21
trans-2-Hexene	0.94	0.79	1.20
2,2-dimethylbutane	0.93	0.77	1.21
2-Methylhexane	0.87	0.64	1.36
1-Pentene	0.85	0.87	0.99
Total	83.56	76.50	
Average			1.09

Table D-20. Measured vs TEVAP-Predicted Speciation Profiles: Expt.8 Hot Soak Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Butane	28.51	2.02	14.12
Isopentane	20.42	32.85	0.62
MTBE	8.66	9.12	0.95
n-Pentane	7.33	11.32	0.65
2-Methylpentane	3.55	4.79	0.74
trans-2-Pentene	2.71	4.55	0.60
Toluene	2.65	1.34	1.97
3-Methylpentane	1.79	2.38	0.75
2-methyl-2-butene	1.38	2.21	0.62
n-Hexane	1.28	1.61	0.80
Methylcyclopentane	1.17	1.35	0.87
cis-2-Pentene	1.11	2.06	0.54
Benzene	1.06	0.85	1.25
t-2-butene	0.78	1.55	0.50
m-Xylene	0.65	0.20	3.25
1-Hexene	0.64	0.83	0.77
trans-2-Hexene	0.62	0.79	0.79
2,3-Dimethylbutane	0.62	2.59	0.24
2-Methylhexane	0.58	0.64	0.91
cis-2-Butene	0.53	1.14	0.47
Total	86.04	84.18	
Average			1.02

Table D-21. Measured vs TEVAP-Predicted Speciation Profiles: Expt.8 Diurnal Results

	Percent by Mass		
Compound	Measured	Predicted	Meas/Pred
Isopentane	31.68	32.73	0.97
n-Pentane	12.27	11.11	1.10
MTBE	11.40	8.64	1.32
2-Methylpentane	5.12	4.50	1.14
trans-2-Pentene	4.40	4.46	0.99
3-Methylpentane	2.50	2.22	1.12
2-methyl-2-butene	2.08	2.16	0.96
cis-2-Pentene	1.95	2.02	0.96
Butane	1.86	2.12	0.88
n-Hexane	1.67	1.49	1.12
Toluene	1.55	1.15	1.35
t-2-butene	1.46	1.61	0.91
Methylcyclopentane	1.32	1.24	1.07
cis-2-Butene	1.00	1.19	0.84
Benzene	0.90	0.77	1.16
2,2-dimethylbutane	0.84	0.73	1.15
1-Hexene	0.83	0.78	1.06
Cyclopentane	0.82	0.00	
2,3-Dimethylbutane	0.82	2.44	0.33
1-Pentene	0.79	0.86	0.92
Total	85.27	82.23	
Average			1.04

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